Science Technology National Nuclear Security Administration's Lawrence Livermore National Laboratory University Relations regram A collection of articles reprinted from Science & Technology Review. UCRL-TR-224024

About the Cover

Lawrence Livermore's Student Employee Graduate Research Fellowship Program provides University of California (UC) graduate students the opportunity to conduct research at the Laboratory while earning their Ph.D.s. The students apply to the program as a team with their university thesis advisor and a Laboratory mentor. They work on fundamental science in diverse areas across the Laboratory. On the cover, UC Berkeley student Ionel Dragos Hau holds a lithium fluoride crystal similar to one he and his Laboratory mentor, Stephan Friedrich, use for a neutron spectrometer.



Cover design: Amy Henke





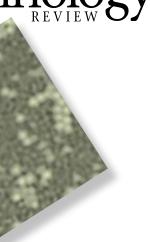


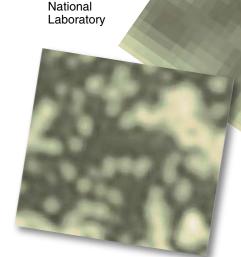


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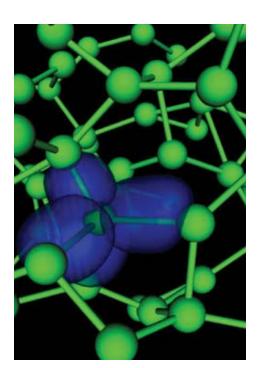




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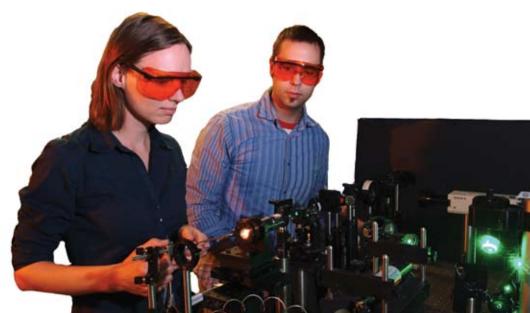
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Collaborative Research Prepares Our Next-Generation Scientists and Engineers

As a Department of Energy multiprogram laboratory, Lawrence Livermore National Laboratory is expanding its expertise related to nonproliferation, biotechnology and health, homeland security, energy, and the environment. Because other institutions have expertise in these fields, Livermore scientists and engineers engage in multiple collaborative efforts in order to maximize the power of the combined talent in solving problems of national importance.

In 1995, Livermore formed its University Relations Program (URP) to facilitate the growing number of collaborations between the Laboratory's researchers and the broader scientific community. URP supports a range of programs that improve access to the Laboratory, contribute to science education, strengthen existing Laboratory programs, and develop new initiatives to facilitate the exchange of expertise among Livermore researchers and their collaborative partners.

Significant strategic collaborations have been formed with university partners. The first article in this reprint issue, "The Power of Partnership," highlights strategic collaborations between the Laboratory and the University of California (UC), as well as other partners. Three particularly strong joint endeavors include the National Science Foundation (NSF) Center for Adaptive Optics at UC Santa Cruz, the NSF Center for Biophotonic Science and Technology with UC Davis, and the National Cancer Center at UC Davis.

URP also serves as a focal point for strategic recruiting programs designed to attract young scientific and engineering talent to Livermore. An integral component of the Laboratory's plan for continually invigorating science and technology at Livermore is recruiting outstanding new scientists and engineers. One of the Laboratory's proven vehicles for providing tomorrow's workforce and for maintaining intellectual vitality is the Student Employee Graduate Research Fellowship (SEGRF) Program. For more than 40 years, SEGRF has provided students the opportunity to work part-time at the Laboratory while completing their dissertations.

The article entitled "Next-Generation Scientists and Engineers Tap Lab's Resources" describes some of the fundamental research conducted by several current and former SEGRF students. Students apply as a team that includes their UC academic advisor and a Laboratory technical mentor. They

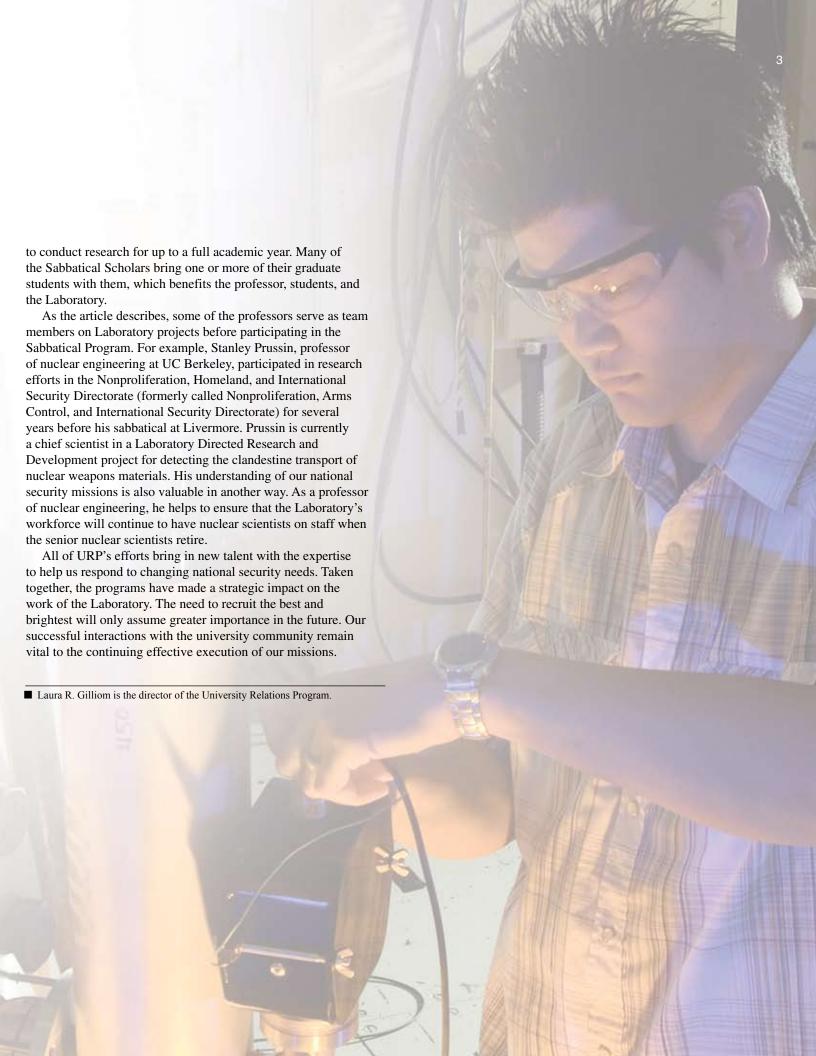
work with scientists and engineers across the directorates, from the National Ignition Facility Programs to Chemistry and Materials Science to Biosciences, in disciplines ranging from optical materials to detectors to advanced simulations. Some UC faculty have developed ongoing collaborations that provide a continuing flow of high-quality students, strengthening the Lab's partnership with their campuses. Livermore scientists and engineers benefit from the students' intellectual vitality and the fundamental research they conduct.

To help persuade the best and brightest to come to Livermore, URP initiated the Lawrence Livermore Fellowship Program in 1997. This prestigious opportunity attracts some of the most sought-after recent Ph.D.s in the world. The criteria for acceptance is extremely rigorous. However, Lawrence fellows are given the opportunity to select the group in which they want to work and the freedom to conduct research in an atmosphere that cultivates their creativity. They also often grow to become our next-generation scientific leaders.

The article entitled "The Best and the Brightest Come to Livermore" describes some of the Laboratory's discoveries that were possible because of these Lawrence fellows. They help Livermore build new theoretical and experimental capabilities, keeping the Laboratory at the forefront of science and engineering. Often, they set new directions. For example, the Biosciences Directorate's BioSecurity and Nanosciences Laboratory was invigorated by Lawrence fellows who brought new techniques that hadn't previously existed at Livermore. Some of the work initiated by these fellows is helping to drive our ongoing research relevant to homeland security.

Many Lawrence fellows remain at Livermore after their threeyear fellowship appointment. Those who don't remain, become ambassadors for the Laboratory. In particular, those who have become professors at top universities, such as MIT, Stanford, and UCLA, provide an ongoing pool of talent and established collaboration for our research programs.

Another URP program that strengthens research projects between faculty and their graduate students is the Sabbatical Scholars Program. The article "Faculty on Sabbatical Find a Good Home at Livermore" highlights some of the results from this program. Initiated in 2000, it has already provided approximately 30 faculty members access to Livermore's facilities



The Power of

Strategic collaborations between Lawrence Livermore and other University

ISTITUTIONS that conduct similar or complementary research often excel through collaboration. Indeed, much of Lawrence Livermore's research involves collaboration with other institutions, including universities, other national laboratories, government agencies, and private industry. In particular, Livermore's strategic collaborations with other University of California (UC) campuses have proven exceptionally successful in combining basic science and applied multidisciplinary research. In joint projects, the collaborating institutions benefit from sharing expertise and resources as they work toward their distinctive missions in education, research, and public service.

As Laboratory scientists and engineers identify resources needed to conduct their work, they often turn to university researchers with complementary expertise. Successful projects can expand in scope to include additional scientists and engineers both from the Laboratory and from UC, and these projects may become an important element of the research portfolios of the cognizant Livermore directorate and the university department. Additional funding may be provided to broaden or deepen a research project or perhaps develop it for transfer to the private sector for commercial release.

Occasionally, joint projects evolve into a strategic collaboration at the institutional

level, attracting the attention of the Laboratory director and the UC chancellor. Government agencies or private industries may contribute funding in recognition of the potential payoff of the joint research, and a center may be established at one of the UC campuses. Livermore scientists and engineers and UC faculty are recruited to these centers to focus on a particular area and achieve goals through interdisciplinary research. Some of these researchers hold multilocation appointments, allowing them to work at Livermore and another UC campus. Such centers also attract postdoctoral researchers and graduate students pursuing careers in the centers' specialized areas of science.

of California campuses strengthen basic science research and national security.

Another method Livermore uses to foster university collaboration is through the Laboratory's institutes, which have been established to focus university outreach efforts in fields of scientific importance to Livermore's programs and missions. Some of these joint projects may grow to the level of a strategic collaboration. Others may assist in Livermore's national security mission; provide a recruiting pipeline from universities to the Laboratory; or enhance university interactions and the vitality of Livermore's science and technology environment through seminars, workshops, and visitor programs.

Supporting Collaborative Growth

In 1995, Livermore formed its University Relations Program (URP) to facilitate the growing number of collaborations between the Laboratory's researchers and UC faculty. Working with the UC Office of the President (UCOP), URP supports a broad range of programs that improve access to Livermore, contribute to science education (see the box on p. 16), strengthen existing Laboratory programs, and develop new initiatives to facilitate the exchange of expertise among Livermore researchers and university faculty. URP is also assisting in program development for UC's newest campus, UC Merced. (See the box on p. 11.)

Program director Laura Gilliom says, "URP's role, in partnership with the Laboratory's directorates, is to broaden and deepen our levels of interaction with universities. Our strategic-level collaborations with other UC campuses have brought enormous benefits to the Laboratory and to UC. We're also working to enable strategic collaborations with other universities."

URP oversees the six Livermore institutes that have been established in specific fields. Much of the work performed by the institutes is inspired by work originally developed to fulfill the Laboratory's national security missions. And even as joint research advances are

Edward Teller's Education Vision

Livermore's University Relations Program (URP) manages educational programs for kindergarten through graduate school. The programs continue the vision established by Edward Teller, who began his 60-year teaching career in 1934. When asked what scientists could do to help the public overcome their suspicions about new technology and science, Teller responded, "It is not up to the scientists. It is up to teachers."

Teller had a vision to create an educational department at Livermore that would operate as part of the College of Engineering at the University of California (UC) at Davis. In 1963, the Department of Applied Science (DAS) was established. Professors from the university and scientists from the Laboratory have since provided classroom instruction and hands-on experience with Laboratory projects to more than 1,400 M.S. and Ph.D. students.

Livermore expanded its education efforts with the Science and Technology Education Program (STEP), which provides professional development instruction for science teachers and enrichment programs for students. STEP events are aligned with science content standards for California public schools and the California standards for teaching. Livermore scientists identify Laboratory areas that best align with the instructional content of the programs. STEP disseminates the programs through the Edward Teller Education Center,

a UC-sponsored professional development center for science teachers.

The Critical Skills Internship Program facilitates undergraduate research interactions with the Laboratory by matching college students with internships within Livermore's Stockpile Stewardship Program. Most of these internships are funded directly by the National Nuclear Security Administration.

Livermore also has a few programs designed to help train and recruit college graduates. The Research Collaborations Program (RCP) links Laboratory

Livermore scientist Robert Tebbs (far left) and Michele Bennett (second from right, now at the National Institutes of Health) mentor faculty interns from Merced College. The interns worked with the Laboratory to update their knowledge of biotechnology for classroom instruction.

scientists with professors, postdoctoral researchers, and students at historically black colleges and universities and minority institutions. RCP has developed 24 technical collaborations connecting the Laboratory with 15 minority universities. The Student Employee Graduate Research Fellowship (SEGRF) Program grants fellowships to Ph.D. candidates from UC. There are currently 60 SEGRF students at Livermore.

Finally, the Lawrence Livermore Postdoctoral Fellowship Program, known informally as the Lawrence Fellowship, is a tribute to Nobel laureate and Laboratory cofounder Ernest O. Lawrence. Researchers are hired by the Director's Office in cooperation with URP. The criteria for acceptance are rigorous. In the first four years of the program, only 15 of 1,849 applicants were accepted as Lawrence fellows. (See S&TR, November 2002, pp. 12-18.)

In a survey conducted by Science magazine early this year, postdoctoral researchers ranked Livermore the seventh best place for postdoctoral researchers to work, from a pool of 61 U.S. institutions. URP director Laura Gilliom says, "The postdoctoral researchers who come here know they will be able to do cuttingedge research using the world's most advanced lasers, accelerator mass spectroscopy, and nuclear magnetic resonance spectroscopy tools, and couple experimental and computational science."



applied to human health, the environment, and other areas of importance, the technologies continue to support the nation's security.

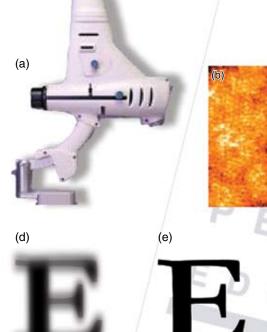
Adapting Adaptive Optics

Livermore's first institute, the Institute of Geophysics and Planetary Physics (IGPP), was founded in 1982, with Livermore astrophysicist Claire Max serving as the first IGPP director. The Laboratory's branch of IGPP is linked to units on several campuses and is known as one of the leading geoscience and astrophysical research centers in the world.

IGPP's astrophysics efforts first received wide recognition through the MACHO (Massively Compact Halo Objects) project. Originally funded by Livermore's Laboratory Directed Research and Development (LDRD) Program, that project was a digital imaging study in search of cosmic dark matter. (See E&TR, April 1994, pp. 7–17; *S&TR*, April 1996, pp. 6–11.) Later, IGPP received LDRD funding to develop adaptive optics for ground-based telescopes. Adaptive optics systems measure the distortion of light from a star and then remove the distortion by reflecting the light off a deformable mirror that adjusts several hundred times per second to sharpen the image.

In 1995, Livermore installed a laser guide star—an artificial guide star system with adaptive optics—on the Shane Telescope at UC's Lick Observatory on Mount Hamilton in California. (See S&TR, July/August 1999, pp. 12-19; June 2002, pp. 12-19.) Shane was the first major astronomical telescope to use this system. In 2001, a similar system was installed on the Keck II Telescope in Hawaii, which is operated jointly by UC, the California Institute of Technology (Caltech), and the National Aeronautics and Space Administration (NASA).

In 2001, UC also opened the Center for Adaptive Optics at UC Santa Cruz. Funded by the National Science Foundation (NSF),



(a) An adaptive optics phoropter can be used to correct eyesight aberrations and will allow ophthalmologists to view certain types of individual retinal cells for the first time. The effects of adaptive optics correction are shown on single cells in the human retina and the E from a standard eye chart: (b, d) before correction and (c, e) after correction.

the center's 27 partnering institutions include several UC campuses, Caltech, the University of Chicago, the University of Rochester, four laboratories, and 15 other partners. The center coordinates the efforts of researchers across the country involved in adaptive optics for astronomical and vision science. Max, who is deputy director of the center, says, "The Center for Adaptive Optics allowed Livermore to branch out from astronomy and lasers and apply adaptive optics to vision science, homeland security, and other developing applications."

In one LDRD-funded project, adaptive optics systems are being developed to correct for eye aberrations, detect the onset of eye diseases, and increase vision beyond 20/20. Livermore optical physicist Scot Olivier, who is an associate director of the center, leads a team that is partnering with the UC Davis Medical Center and the University of Rochester to apply this technology to three types of imaging systems. The instruments, which will increase resolution over existing instruments by a factor of three, are being designed to allow ophthalmologists to view certain types of individual retinal cells for the first time. In 2003, one of the

instruments, the microelectromechanical systems- (MEMS-) based adaptive optics phoropter, received an R&D 100 Award. (See *S&TR*, October 2003, pp. 12–13.)

Glasses and contacts can correct for two eyesight aberrations: focus, which causes farsightedness or nearsightedness, and astigmatism. Adding adaptive optics to diagnostic instruments will allow optometrists to correct other types of aberrations. This capability will help specialists in prescribing new vision correction procedures such as custom laser refractive surgery. Ophthalmologists can use it to resolve eye cells as small as 2 to 3 micrometers, allowing them to detect diseases such as macular degeneration and glaucoma at an early stage. Physicians will also be able to monitor the effectiveness of drug treatments more closely.

Olivier believes that with adaptive optics, most people can achieve 20/10 or even 20/8 vision. "20/20 is just the average vision that can be corrected by glasses," he says. "Perfect vision would be limited only by the size of the pupil, or diffraction of light, and the ability of the retina and the brain to process the signals." The Department of Energy (DOE) and the National Institutes of

Health (NIH) are funding construction of the adaptive optics imaging systems on diagnostic instruments at the UC Davis Medical Center in Sacramento.

Detecting Faint Planets

The Center for Adaptive Optics continues to be active in astronomy applications, and a recent concept being pursued with LDRD funding is extreme adaptive optics. A team led by IGPP astrophysicist Bruce Macintosh and UC Berkeley professor James Graham is developing an extreme adaptive optics planet imager, which, for the first time, will allow astronomers to make direct images of planets orbiting stars. (See the figure below.)

Currently, astrophysicists infer the presence of a planet by the wobble a star makes, which is caused by the tug of gravity from a planet orbiting the star. The scientists then measure the Doppler shift that occurs as the planet makes a complete orbit around the star, a process that can take a decade or more. The challenge in detecting planets and imaging them

In this simulation of an extreme adaptive optics system, scattered light from a bright star spills out from behind the dark occulting spot. The adaptive optics system clarifies a dark-hole region, showing a planet (circled) four times the mass of Jupiter.

Occulting spot Planet 2 arcseconds

directly has been that the light from a star is a billion times brighter than the planet orbiting it, making the planet nearly impossible to see. The planets are also 10 million to 1 billion times smaller than their stars. "Existing systems were designed to detect faint objects such as galaxies, and a laser guide star was needed for that," Macintosh says. "Our goal is to image planets next to the bright, scattered light surrounding a natural star."

To discern the faint planets, the team is using MEMS technology to reduce the size of the actuators so that 4,096 actuators can fit on a deformable mirror. By contrast, Lick's system has 127 actuators, and Keck II has 349. With this extreme adaptive optics system, astronomers will no longer need to wait until a planet completes an orbit. Instead, they will be able to see planets far from the star and take measurements of the planets directly.

Livermore and UC Santa Cruz will build an extreme adaptive optics system, and UC Los Angeles is building the spectrometer. NASA's Jet Propulsion

Laboratory is providing its expertise in calibrating precision optics. The system could be installed on a telescope by 2008.

Macintosh says the data from this system will be important because scientists still do not understand how a solar system forms. "We think planets are formed in the outer regions of the solar system and move inward," he says, "but being able to study them directly will provide us with more complete answers."

Max adds that applications of adaptive optics extend beyond astronomy and vision science. "The amazing thing is that, as a result of our work in adaptive optics to help astronomy, Livermore is also doing adaptive optics work for homeland security, surveillance, and projects for DARPA" (the Defense Advanced Research Projects Agency).

Analyzing Tiny Samples Fast

Many UC projects take advantage of Livermore's tools to advance their work. One frequently used technology is accelerator mass spectrometry (AMS). AMS is an ultrasensitive technique that measures the concentrations of specific isotopes in samples weighing less than 1 milligram. The process is fast, producing results in days compared with other techniques that can take months.

In 1989, Livermore established its Center for Accelerator Mass Spectrometry (CAMS) to diagnose fission products from nuclear tests and study climate and geologic records. At the time, UC did not have AMS capability. Livermore physicist Jay Davis worked with UCOP for initial funding to help support CAMS. In exchange, UC researchers were allotted a percentage of time with the center's spectrometer. The success of CAMS led to the center becoming a joint UC-Livermore facility, and it is now an established institute.

During the past decade, CAMS scientists have worked with university collaborators to develop analytic approaches that will define environmental and biochemical processes. They have



applied this expertise to research ranging from national security to global climate cycles to biomedicine. The facility has become an important resource to researchers at the UC Davis Cancer Center, which combines Livermore's science, medical technology, and engineering expertise with UC Davis's expertise in cancer research and clinical medicine.

Vitamin Activity in Humans

Early on, CAMS scientists worked with UC collaborators to create an entirely new application of AMS—following isotopically labeled compounds at trace doses through cells from human subjects. Livermore physicist John Vogel received funding from UC and LDRD for his pioneering work in nutrition research, which was instrumental in establishing CAMS for biomedical applications. In 1999, NIH designated CAMS as its only National Research Resource for biological AMS. Worldwide, CAMS is one of the few AMS facilities working on biomedical and pharmaceutical applications. (See S&TR, November 1997, pp. 4–11; July/August 2000, pp. 12–19.)

Vogel, who is also an adjunct professor of nutrition at UC Davis, is collaborating with Andrew Clifford, a UC Davis professor of nutrition, to determine whether the recommended dietary allowance (RDA) for vitamins is appropriate for all people. RDAs are currently set by epidemiological studies, which involve determining the cause of a disease once it has occurred. AMS allows researchers to examine vitamins' physiological activity in the body—that is, how vitamins are interacting in the body in real time.

Vogel and Clifford first studied folate, a vitamin that is important for heart health and preventing birth defects. They tracked 13 people with a median age of 24 years—the first folate study to focus on this age population. Tracking this age group has been difficult in the past. Although stable isotopes can be used to track folate, high doses must be given, preventing an accurate picture of the vitamin's activity. Radioisotopes can also be used to track a vitamin, but they give off radiation. Early tests using radioisotopes such as carbon-14

were done on elderly cancer patients, which is not the ideal group for studying dietary requirement levels to prevent birth defects.

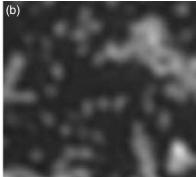
The biggest surprise from the team's results, which will appear soon in the *American Journal of Clinical Nutrition*, was that a large amount of folate is recycled in the body and still present seven months after ingestion. The team will next study other populations to compare results.

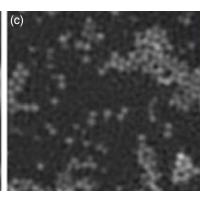
Another study focused on vitamin A metabolism in six women in their twenties. The team's goal was to determine if a sufficient amount of the vitamin stored in the body modifies the need for betacarotene, which converts to vitamin A. Results showed that even with sufficient vitamin A stores, adding beta-carotene allowed better absorption and less excretion of beta-carotene. The team's hypothesis is that vitamin A improved the health of the intestines, so absorption of both vitamin A and beta-carotene improved.

Vogel says, "An epidemiological study might conclude that if people have enough vitamin A, they don't need more

Micrographs of fluorescent plastic balls, each 50 nanometers in diameter, show the improved resolution that researchers hope to achieve with living cells: (a) conventional microscopy, (b) linear structured illumination microscopy, and (c) saturated structured illumination microscopy.







beta-carotene. But a physiological study, which can be done using AMS, shows that vitamin A allows beta-carotene to be processed more efficiently, and we see a cascade of events going on in the body. The added beta-carotene also improves antioxidant stores even if it is not needed to make vitamin A. What's more, AMS's sensitivity means researchers don't have to worry about radiation exposures."

Clues to Gulf War Illness

Some of Vogel's early toxicology work using AMS is also bringing more understanding to another health issue of national concern. Results from his collaborative studies with UC Davis and UC Riverside on the effects of low-dose exposures of pesticides are helping physicians better understand Gulf War Syndrome.

Two of the most common types of pesticides are organophosphates and pyrethroids. Organophosphates are also related to the nerve gases sarin and VX. Using a carbon-14 tracer, Vogel's team measured the amount of toxin present in mouse brains after low-dose exposure to one pesticide and to two different pesticides together. Tests were also performed with and without the pharmaceutical pyridostigmine bromide (PYB), which was given to U.S. soldiers to protect them from possible exposure to nerve gas.

Although PYB did have an overall protective effect, the exposure to two pesticides increased the amount of toxin

in the brain by 25 to 30 percent, compared with exposure to just one pesticide. For U.S. soldiers, low-dose exposure to nerve gas and subsequent exposure to a pesticide that, for example, controls sand fleas might increase the amount of toxin reaching the brain, even with the ingestion of PYB. In 2003, Vogel presented these findings at a Department of Veterans Affairs research meeting addressing illnesses related to the 1991 Gulf War.

Manipulating Cells with Light

Advances in adaptive optics and AMS are allowing an unprecedented view of living cells. Another emerging area, called biophotonics, uses light and other forms of radiant energy to detect, image, and manipulate biological organisms at the cellular level. Applications of biophotonics include using light to image or selectively treat tumors, sequence DNA, and identify single biomolecules within cells.

The Center for Biophotonics Science and Technology (CBST), which was established at UC Davis in 2002, is the only NSF-funded center in the U.S. devoted to the study of light and radiant energy in biology and medicine. This collaboration brings together about 100 researchers, including physical scientists, life scientists, physicians, and engineers from Livermore; UC Davis, Berkeley, and San Francisco; Stanford University; and other universities.

Livermore physicist and UC Davis professor Dennis Matthews leads CBST

along with UC Davis neurosurgeon Jim Boggan. Matthews says, "If we want to see how a single molecule interacts with other molecules inside a cell under different conditions, we don't have the technology to do that right now. Biophotonics, combined with other technologies we are developing, will allow us to see changes in the living cell."

UC San Francisco is leading a CBST project to develop structured illumination microscopy, an ultrahigh-resolution method to study the inner workings of cells. The method illuminates a sample with a light pattern that mixes with highresolution sample features to produce resolvable low-resolution moiré fringes. (Moiré fringes are interference effects from overlaying two similar patterns, seen for instance when looking through two screen windows or two layers of mesh fabric.) By observing the fringes, the system can computationally reconstruct the original high-resolution information. This effect is pronounced when the illumination pattern is tight. By using tighter patterns, scientists can achieve better resolution than they can by direct illumination. This method, called saturated structured illumination, has produced some of the highest resolution images ever obtained with far-field visible light. (See the figure above.)

Tech Transfer Fills Many Needs

DOE is interested in structured illumination microscopy technology for the Genomics:GTL project, the follow-



The Birth of a University

The University of California (UC) and Lawrence Livermore have entered a new form of strategic collaboration to help establish the newest UC campus, which will be located in the San Joaquin Valley—the most populous region of the state without a UC campus. In 1995, UC chose Merced as the site for the nation's first public research university to be built in the 21st century. When fully developed, the campus will be home to 25,000 students and 6,600 faculty and staff.

The Laboratory's University Relations Program (URP) is helping UC Merced to become an important research university within the UC family, and areas of cooperation were defined in a memorandum of understanding signed on October 6, 2000.

URP's Paul Dickinson coordinates many areas of the collaboration. "Livermore is playing a critical role in recruiting science faculty for Merced," he says. "Faculty candidates visit the Laboratory to meet with potential colleagues, tour facilities, and gain an understanding of how partnering with the Laboratory can help facilitate their professorship at Merced.'

As with other UC campuses, some members of the Merced faculty are expected to have multilocation appointments at Livermore. Laboratory researchers are also being encouraged to have multilocation appointments or become adjunct faculty at Merced.

So far, Merced has hired 27 faculty members, in addition to Maria Pallavicini, the dean of Natural Sciences; Jeff Wright, the dean of Engineering; Kenji Hakuta, the dean of Social Sciences, Humanities, and Arts; and Keith Alley, provost and vice chancellor of Research and dean of Graduate Studies. By August 2005, UC Merced is expected to have 60 faculty members and several adjunct members.

Because Merced is expected to become a valuable source of postdoctoral researchers and employees for the Laboratory, Livermore will offer graduate student internships. The Laboratory is also helping to plan a Central Valley institute that will help increase the number of students eligible to enter the university. Wright says, "Our collaboration with Livermore has been invaluable for building our academic programs, recruiting faculty, and providing future faculty the opportunity to see potential areas of research partnership with the Laboratory."

on to the Human Genome Project. Advanced microscopy, such as structured illumination, will allow researchers to study the function and structure of proteins in microbes. DOE is also funding a project to determine whether microbes can be used to synthesize cells for such applications as creating hydrocarbons for fuel, eliminating diseases in plants, purifying water, and scavenging for radioactive particles.

Another CBST project is using Livermore-developed optical probes with Raman spectroscopy to characterize cell function at the nanometer scale. (See S&TR, May 2004, pp. 4–11.) Raman scattering can identify a molecule by recording its distinct vibrational fingerprints as the molecule scatters laser light. Livermore physicist Tom Huser leads an LDRD-funded team that developed a method called surface-enhanced Raman spectroscopy, in which nanometer-size gold crystals are attached to molecules or cells. This method increases the signal by a factor of a quadrillion (10^{15}) .

The gold nanoparticles, which are about 50 nanometers in diameter, serve as detectors that provide detail about the environment. The particles are covered with molecules of mercaptobenzoic acid, whose Raman spectrum changes with pH. As a cell reacts to external stimuli, its pH

usually changes in response. One possible application of this technique is studying the pH of cancer cells while trying to develop better chemotherapeutics.

Matthews has also set up a program within CBST to develop optical-based medical devices in collaboration with industrial partners and UC campuses. Several technologies have already been transferred to industry for commercial development, including a device for treating ischemic stroke; micropower impulse radar for medical diagnostics; an implantable, continuous glucose monitor; and ultrashortpulse laser microsurgery devices.

The Benefits of Collaboration

Members of the UC faculty have long cited the successful outcomes of their collaborations with Livermore researchers as an important reason to continue institution-to-institution research. Project results often establish a continuum of ideas for faculty to jump-start new research.

UC has two programs that provide grants to support emerging research activities until they become fully funded projects. The Campus-Laboratory Collaborations (CLC) Program funds three-year projects on issues that will affect the state of California. The Campus-Laboratory Exchange Program

supports the exchange of people between campuses and the Laboratory. For example, Livermore geochemist Tom Guilderson leads a CLC-funded project with UC Santa Cruz researchers to define the fate of organic compounds in oceans. Understanding the global carbon cycle is an important research area because oceans serve as major reservoirs for carbon.

These programs not only support emerging technology, says Gilliom, but they also help university researchers gain experience in managing multidisciplinary programs. "Academics traditionally follow a focused career path, and gaining tenure doesn't always require experience as project managers. The interdisciplinary research experience that our scientists and engineers bring helps universities deliver their technologies where they are needed."

Livermore, in turn, greatly benefits from working with the great minds of academia. UC faculty members have won 32 Nobel prizes, and the current UC faculty includes 18 Nobel laureates.

Fostering Innovation

Postdoctoral researchers also provide the Laboratory many benefits. In general, students are up to date in training for their respective fields, know the latest techniques being used, and have fresh ideas



on how to couple different technologies. Postdoctoral researcher Adam Love says, "Postdocs at Livermore want to carve a unique path for themselves. We want to create novel ways to solve problems, which means we fail most of the time. But when we succeed, it's a big deal because it usually results in a breakthrough for an area of science."

Postdoctoral researchers benefit from having access to Livermore's researchers and facilities. "Virtually any instrument we want," says Love, "can be found here at the Laboratory." Love, who earned a Ph.D. in environmental engineering at UC Berkeley, specializes in contaminant transport processes in environmental systems. He received a three-year minigrant for his dissertation on reconstructing environmental levels of tritium by analyzing tree rings, and access to CAMS was key for his research.

Using AMS, Love measured carbon-14 and tritium levels throughout 150-millimeter cores taken from trees at Lawrence Berkeley National Laboratory. Until recently, Lawrence Berkeley used tritium to synthesize the tritium-labeled biological molecules used in tracing experiments. With his AMS results, Love established dates for the core section used in the tritium analysis by matching

carbon-14 levels in the wood with known atmospheric levels. The AMSmeasured tritium levels matched the levels reported by Lawrence Berkeley for the corresponding years over the last 30 years. Thus, he demonstrated an effective new application of AMS for retrospective environmental studies and for its use as a verification tool.

Love says that coming up with measurement-based techniques to reconstruct historical contaminant exposure levels is a fairly novel concept. Having access to CAMS was critical because AMS is the only technique that has both the sensitivity and throughput for running the numerous samples required for high resolution in many reconstruction scenarios. "In retrospective environmental studies," he says, "these capabilities are crucial, especially if we want to do a study going back many decades."

Forging Future Collaborations

Livermore's strategic collaborations to date have been with UC, but URP is also collaborating with other institutions. This year, Laboratory director Michael Anastasio signed a memorandum of understanding to establish a strategic collaboration with the Naval Postgraduate School (NPS). Livermore-NPS collaborations will focus

on joint program development for the Department of Defense.

As the Laboratory increases its number of strategic collaborations with other institutions, UC and Livermore will continue to nourish the relationship they have formed from working together for more than 50 years. "Livermore has powerful, deep, and historic connections with UC," says Anastasio. "Our strategic collaborations have enhanced the quality of the Laboratory's research programs and helped us recruit the best people. These collaborations are good for the Laboratory, good for UC, and good for the nation."

—Gabriele Rennie

Key Words: accelerator mass spectrometry (AMS), adaptive optics, biophotonics, Center for Accelerator Mass Spectrometry (CAMS), Center for Adaptive Optics, Center for Biophotonics Science and Technology (CBST), Institute of Geophysics and Planetary Physics (IGPP), University of California (UC), UC Office of the President (UCOP), University Relations Program (URP).

For further information contact Laura Gilliom (925) 422-9553 (gilliom1@llnl.gov).





A Livermore

Lawrence Livermore National Laboratory



Science (DAS), which was established at the Laboratory by Livermore cofounder Edward Teller in 1964. With a lifelong commitment to science education, Teller recognized the need for a graduate program in applied science. He worked with UC administration to site a universitylevel education facility at the Laboratory and served as the first administrator of DAS. The SEGRF Program has supported students at DAS.

Over the years, graduate education opportunities at Livermore have grown to be broader than the disciplines emphasized in DAS. In 1999, the SEGRF Program opened to all UC Davis departments to meet the Laboratory's need for graduate students in areas such as laser physics, plasma diagnostics, fusion energy, accelerator technology, computational sciences, biosciences, materials science, and environmental and energy sciences. In 2001, the program opened to all UC campuses.

To apply for the SEGRF Program, students must pass their preliminary exams for Ph.D. candidacy, propose a project of interest to the Laboratory, and have a university thesis advisor and a

Laboratory mentor. SEGRF recipients are selected from a pool of applicants by a committee of representatives from all of the Laboratory's directorates. In support of the directorates, Livermore's University Relations Program (URP) manages the SEGRF Program and facilitates interactions with UC campuses.

Paul Dickinson, who manages the SEGRF Program at Livermore, says, "To maintain the Laboratory's scientific and technological excellence, it is essential that we recruit bright, young scientists and engineers." SEGRF participants are half-time Laboratory employees during the academic year and fulltime employees over the summer.

The program has achieved impressive results. Forty-five percent of SEGRF students become Laboratory employees. "Many of the other students go to other national laboratories or universities and collaborate with us on projects or become a resource for recruiting

other students," says

Dickinson.

Cornucopia of Experts

The Laboratory's longtime approach of using multidisciplinary collaborations to solve problems benefits the SEGRF Program. Erica McJimpsey, a UC Davis student and SEGRF participant, says, "I'm working with a team of engineers, biologists, computer scientists, physicists, and chemists, which is an advantage I wouldn't have in an academic environment." For her Ph.D. in analytical chemistry, McJimpsey is writing a dissertation on the characterization of single-particle ionization. She is working with the Laboratory's Bioaerosol Mass Spectrometry Group within the Chemistry and Materials Science Directorate.

In 2001, a Livermore team, originally funded by the Laboratory Directed Research and Development (LDRD) Program, developed the bioaerosol mass spectrometry (BAMS) system—the only instrument that can distinguish between two related but different spore species in less than 1 minute. The mass spectrometer



can also sort out a single spore from thousands of other particles. (See *S&TR*, September 2003, pp. 21–23; October 2005, pp. 8–9.) The BAMS team won a 2005 R&D 100 Award from *R&D Magazine* for developing the instrument. The Department of Defense's (DoD's) Technical Support Working Group and Defense Advanced Research Project Agency funded the Livermore team to develop BAMS for its potential use in identifying biological agents such as anthrax.

McJimpsey is working with the team to extend the spectrometer's capability for identifying signatures of proteins in individual spores. The team is using an ionization technique called matrix-assisted laser desorption ionization (MALDI) to analyze single particles and achieve greater sensitivity. In MALDI, the biomolecule of interest, often a protein, is irradiated with a laser. Because proteins are sensitive to temperature changes and can easily degrade, a chromophore (a molecule that absorbs light) is mixed with the protein to absorb the brunt of the energy from the laser.

Livermore has three BAMS instruments, one of which was modified by McJimpsey and two former SEGRF students, Scott Russell and Gregg Czerwieniec, to conduct the experiments using the MALDI technique. "At the Laboratory," says McJimpsey, "I can apply my passion for instrumentation toward an important homeland security mission." In addition to her professional goal of obtaining a DoD Presidential Management Internship to work on homeland security, McJimpsey also hopes to be a role model and mentor to minorities interested in pursuing careers in science.

In another homeland security effort, Ionel Dragos Hau, a nuclear engineering student at UC Berkeley and SEGRF participant, is working with Livermore's Advanced Detector Group to develop a novel type of neutron spectrometer as part of his thesis on neutron detection. One advantage of this neutron spectrometer is



Laboratory postdoctoral researcher Faranak Nekoogar conducts research in ultrawideband radio-frequency identification systems.

that its sensitivity is so high it can detect light elements, such as oxygen, within a heavy matrix such as plutonium. It can also detect nuclear material behind a heavy metal that would shield other types of radiation such as gamma rays. For example, if nuclear material were concealed in a lead object, the material's neutrons would interact with the lead and scatter in ways that provide a signature identifiable to the neutron spectrometer. The team uses lithium fluoride for the detector material because large crystals of it can be grown; the greater the size of the crystal, the greater the capability to detect neutrons.

Unlike spectrometers that collect electrical charges, this neutron detector collects heat in the form of phonons produced from a neutron reaction. A thermometer measures the rapid increase in heat, and the source of the nuclear material is revealed by the strength of the heat signal. However, because the heat has to flow out of the detector after each neutron interaction before another count

can be taken, and phonons travel more slowly than electrons, the count rate is comparably lower than some types of gamma-ray detectors. Hau is working with the Livermore team to improve the spectrometer's count rate.

Researchers, Authors, and Inventors

Livermore scientists and engineers benefit from the students' intellectual vitality and the fundamental research they conduct. The students greatly contribute to work that is publishable in papers, an important part of both the student's and the Laboratory scientist's career development. Some of the SEGRF students are well-seasoned authors by the time they complete their Ph.D.s. In addition to publishing articles on ultrawideband (UWB) communications, former SEGRF student Faranak Nekoogar, now a postdoctoral researcher in the Engineering Directorate, published two technical books and filed eight patents or records of inventions before completing her Ph D

UWB communication is fundamentally different from conventional communication systems because it employs extremely narrow (picoseconds to nanoseconds) radio-frequency pulses to communicate between transmitter and receiver. (See *S&TR*, September 2004, pp. 12–19.) Using short-duration pulses rather than continuous waveforms offers several advantages over traditional wireless technologies. They include large throughput, covertness, tamper-resistance to jamming, low transmit power, and the ability to coexist with current radio services.

A very low-power UWB radar system called micropower impulse radar (MIR) was invented in 1993 by Livermore electronics engineer Tom McEwan. It has been one of the most commercially successful licensed inventions both at Livermore and throughout the Department of Energy (DOE). Livermore won R&D 100 awards for two of the technologies that use MIR—an electronic dipstick (S&TR, October 1996, pp. 16–17) and a bridge inspection system (S&TR, October 1998, pp. 7–8). The Laboratory holds 30 MIR patents and patent filings, with Nekoogar's among them.

UWB pulses are safe to use around people and do not interfere with computers, digital watches, cellular phones, or radio and television signals. UWB technology could replace the interface between computers, printers, and entertainment devices in homes, providing a wireless network of integrated systems. Nekoogar says UWB technology could also overcome the power and range limitations of the current radio-frequency identification systems, providing more reliable monitoring of assets and people. In addition, it has potential use in tracking applications to prevent cargo-container tampering, provide situational awareness for soldiers, and help find lost children.

DoD and the Department of Homeland Security are interested in UWB technology for covert communications in mission critical applications. Nekoogar wrote her thesis on the use of UWB transmittedreference (TR) methods that enable reliable wireless communications in harsh radio propagation conditions. For example, in the heavy metallic environment inside a ship, where conventional wireless technologies fail because multiple reflections of radio signals interfere with each other.

Ultrawideband signals have several advantages, including low transmit power requirements, resistance to interference, and the ability to coexist with other frequencies. Narrowband (30 kilohertz) Wideband (5 megahertz) Ultrawideband (several gigahertz)

Frequency

Nekoogar says the next step will be designing chips to carry UWB-TR systems. "We want to partner with industries that specialize in chip design." Chip design is the subject of the second book Nekoogar has authored; her first book describes the fundamentals of UWB communications.

Partnering with Industry

SEGRF students also have opportunities to partner with industry. As part of Nick Killingsworth's thesis on combustion control in homogenous charge compression ignition (HCCI) engines, the UC San Diego student works with Livermore engineers on an HCCI engine. "I had been studying HCCI technology at UC San Diego and, in particular, combustion control issues," says Killingsworth. "One day, I received an advertisement about the SEGRF Program. It was perfect timing. I contacted the Livermore team right away."

Caterpillar Inc. donated a six-cylinder, spark-ignited (SI) engine, which the Livermore team is converting to an HCCI engine in exchange for providing the company with research data. (See S&TR, April 2004, pp. 17–19.) The research is funded by the California Energy Commission's Advanced Reciprocating Internal Combustion Engine Program and DOE's Office of Energy Efficiency and Renewable Energy.

Combustion in HCCI engines is fundamentally different from that in SI and diesel engines. HCCI combustion involves thermal auto-ignition of a premixed fuel-air mixture, without the flame propagation found in SI engines or the mixing-controlled combustion found in diesel engines. HCCI engines can run extremely lean (low percentage of fuel and a high percentage of air), and the combustion temperature is low enough that the engine produces extremely low nitrogen oxide emissions (a few parts per million). Lean, premixed combustion also results in nearly zero particulate matter emissions.

However, HCCI engines present challenges that have kept them from commercialization. The main hurdles are combustion-timing control, low power output, and difficulty in starting when cold. At cold start, the compressedgas temperature in an HCCI engine is low because the charge receives no preheating from the intake manifold and the compressed charge is rapidly cooled by heat transfer to the cold combustion chamber walls.

The Livermore team's novel solution is to start the engine directly in HCCI mode by preheating the intake with a gasfired burner. Running the intake charge through the preheater while simultaneously spinning the engine with an air starter enables the HCCI engine to achieve ignition. After ignition, the combustion

The HCCI engine does not have a combustion trigger such as a spark plug or fuel injector. Instead, combustion is achieved by controlling the temperature, pressure, and composition of the fuel-air mixture. Multiple-cylinder engines pose an additional challenge because differences in pressure, temperature, and compression ratio invariably exist between the cylinders.

To address this problem, the Livermore team developed a thermal management system in which a controller detects

cylinder-to-cylinder differences and adjusts the intake temperature of each cylinder for optimal combustion timing. Killingsworth is developing the control algorithms to regulate the opening and closing of the cylinders' valves.

The team plans to use the engine as a test bed for HCCI studies. HCCI technology can considerably improve fuel efficiency while providing unmatched flexibility in operating temperatures. At the same time, the technology will meet the stricter

UC San Diego student Nick Killingsworth (center) and his Laboratory mentors Daniel Flowers (left) and Salvador Aceves (right) are converting a Caterpillar spark-ignited engine to a homogenous charge compression ignition engine.



California standards for nitrogen oxide emissions, which go into effect next year.

Combining Talent for a Common Goal

Occasionally, former and present SEGRF students work together as a research team. Physicists Wren Carr and John Adams, both former SEGRF students and now Laboratory employees, are working with UC Davis SEGRF participant Paul DeMange. The team is conducting research relevant to the National Ignition Facility (NIF), the world's most energetic laser being constructed for the National Nuclear Security Administration's Stockpile Stewardship Program. (See *S&TR*, September 2002, pp. 20–29.)

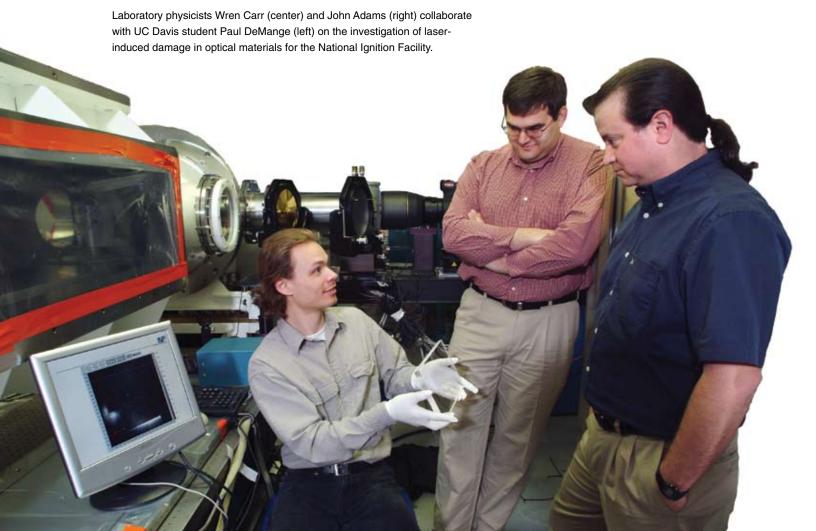
DeMange is investigating the fundamental processes associated with laser-induced damage in optical materials. His experiments have already led to five coauthored publications in journals such as Applied Physics Letters and Optics

Letters. Many of DeMange's research experiments were performed using new instruments that he and Carr built to provide rapid, quantitative measurements of the density of damage sites in crystals.

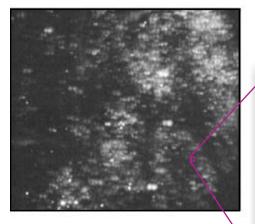
DeMange's early experiments investigated the effects of using different wavelengths to condition potassium dihydrogen phosphate crystals such as those used in NIF. Conditioning is the process of increasing a crystal's resistance to laser-induced damage by pre-exposing the crystal to subdamaging laser intensities. DeMange's results showed that the effectiveness of conditioning is sensitive to the wavelength of the laser light used, with shorter wavelengths providing a better level of conditioning. He also confirmed that exposure to two pulses of different wavelengths simultaneously resulted in more damage than that resulting from exposure to each wavelength separately.

Adams received his Ph.D. through DAS in 2002. While a SEGRF student, he discovered a widely tunable midinfrared laser material that has potential applications for remote sensing of a variety of atmospheric-borne chemicals. He also discovered a new electrooptic material for use at wavelengths near 1 micrometer, for which he earned a patent, and a new frequency-conversion material. Adams recalls being struck by the wealth of knowledge available to him as a student. "The Laboratory is so full of top-notch people that I can't imagine a better environment for a budding Ph.D. If I had a question while reading a journal article, I could often walk down the hall and ask the lead author for clarification. Or, if a piece of equipment broke, an expert was always around to help me. To have access to these resources as a student was phenomenal."

Adams and DeMange's studies are providing Carr with data he needs as







A scanning electron microscope image of a crystal shows the damage imprint left by a laser beam.

principal investigator for a \$1.5 million LDRD project studying conditioning in crystals to mitigate laser-induced damage. Carr says, "Part of the purpose of the LDRD effort is to better understand the laser parameters that govern conditioning of crystals." His work has focused on studying the mechanisms involved in energy deposition by low-intensity, visible, and near-ultraviolet laser light in a material, the mechanisms that govern laser-induced damage, laser machining, and laser conditioning.

While a SEGRF student, Carr demonstrated that damage induced by a laser pulse a few nanoseconds long results in a tiny region inside the crystal reaching a temperature of 12,000 kelvins and a pressure of 250,000 atmospheres of pressure, far higher than had been theorized. The damage sites, which are only a few micrometers in diameter, were examined using a scanning electron microscope and were found to have the same general structure of craters made by underground explosions with 20 orders of magnitude more energy.

Are Diamonds Really Forever?

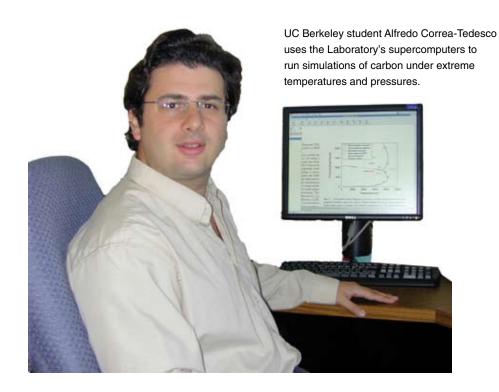
Laser-induced damage in optical materials is one example of modifications that result from extreme conditions. Studying materials exposed to extreme conditions often requires the use of simulations. SEGRF students have

opportunities to conduct research using some of the fastest supercomputers in the world. Alfredo Correa-Tedesco, a theoretical physics student at UC Berkeley, uses the Laboratory's 11-teraops (trillion operations per second) Multiprogrammatic Capability

Resource (MCR) and 23-teraops Thunder machines to run three-dimensional simulations of carbon at high pressures and temperatures. Correa-Tedesco's work is part of a study to determine carbon's phase diagram.

Carbon is one of the most abundant elements in the universe. In its elemental form, carbon is found in coal, graphite. diamond, bucky balls, and nanotubes. These are materials with very different properties, yet at the microscopic level, they differ only by the geometric arrangements of atoms. Little is known about the phase boundaries and melting properties between different crystalline phases of carbon and liquid carbon. Experimental data are scarce because of difficulties in reaching a million atmospheres of pressure and thousands of kelvins in the laboratory.

Correa-Tedesco uses Qbox, a first-principles code developed by physicist François Gygi, formerly at Livermore and now at UC Davis. Qbox can simulate hundreds of atoms at a time



and allows the team to model the transition between two phases in a single simulation cell. "Modeling the coexistence of two phases is difficult," says Correa-Tedesco. "We need the supercomputing capabilities of MCR and Thunder. It takes three to four days and 400 processors of MCR for results, but it could take a year or more for such a simulation without them."

The team determined the solid-liquid and solid-solid phase boundaries of carbon for pressures up to 20 million atmospheres and more than 10,000 kelvins. "We expected to determine just the melting transition for one solid phase," says Correa-Tedesco. "Instead, we found the melting transitions for two solid phases of carbon and the transition between two phases of solid." The results will help researchers devise models of Neptune and Uranus, including an estimate of the planets' core temperatures.

The results will also provide valuable data for experimental studies used to characterize materials at extreme pressures. One of the experimental methods involves using a diamond anvil cell (DAC), which is a small mechanical press that forces together two brilliant-cut diamond anvils.

(See *S&TR*, December 2004, pp. 4–11.) The diamond tips press on a microgram sample of a material to create extremely high pressures. Diamonds are used because they are the hardest known solid and can withstand ultrahigh pressures. They also permit x rays and visible light to pass unhampered through their crystalline structure.

Because diamond is a form of carbon, understanding phase transitions of carbon provides insight on diamonds used in DAC. "Experimentalists are interested in knowing the limits of diamond, for example, at what temperature and pressure the diamond will be destroyed," says Correa-Tedesco. "They also want to know other characteristics about diamond, such as whether it becomes conducting at high temperatures."

The team discovered that diamond remains insulating—that is, resistant to the movement of its electrons-in the solid phase, while it metallizes at melting. Under extreme pressures, certain electrons, which are normally tightly held within an atom's inner electron bands or shells, can move about, resulting in changes in material properties and molecular structures. The

transition is marked by a reduction in the sample's volume as the crystalline lattice shifts to accommodate the new electronic configuration.

Resolving Theoretical Mysteries

Two SEGRF students from UC Davis, Brian Maddox and Amy Lazicki, are combining a DAC with x-ray diffraction techniques to study the effects of pressure on the electronic structure of certain materials during the phase transitions. Maddox works in the Physics and Advanced Technologies Directorate studying transition metal compounds, such as manganese oxide, and rare-earth metals, such as the lanthanides cerium, gadolinium, and praseodymium, all of which exhibit large volume collapses at high pressure. The lanthanides are important to study because the same volume shrinkage occurs in the actinides, which are the elements belonging to the row in the periodic table below the lanthanides and include the nuclear weapon metals plutonium and uranium.

Maddox says, "When we apply pressure to cerium, its volume shrinks by about 17 percent. However, the structure of the material doesn't change. As we move along the row of elements in the periodic



Maddox conducts his experiments using elastic x-ray scattering techniques, such as angle-dispersive x-ray diffraction (ADXRD), and inelastic x-ray scattering techniques, such as x-ray emission spectroscopy and resonant inelastic x-ray scattering. For many years, researchers have conducted inelastic scattering experiments on large samples at room temperature. However, until advancements were made in the synchrotron—a particle accelerator that boosts the velocity of electrons to nearly the speed of light—the techniques could not be applied to high-pressure samples inside a DAC. In ADXRD experiments, researchers send a beam of highly focused x rays through a sample in the DAC and record the diffraction pattern on an image plate detector, which is sensitive to x rays. Changes in the diffraction pattern reveal how a material's structure responds to pressure. Maddox used the synchrotron at Argonne National Laboratory's Advanced Photon Source (APS) to conduct his experiments on manganese oxide. The results showed a transition at

300 kelvins and 1.07 million atmospheres of presure. "These results confirmed that the compound exhibits similarities to transitions in the lanthanides and actinides as has been predicted," says Maddox.

Lazicki also uses the APS synchrotron and a DAC to conduct ADXRD and x-ray Raman spectroscopy experiments on lithium compounds, such as lithium oxide and lithium nitride, which are analogs to hydrogen-containing materials. X-ray diffraction techniques, including ADXRD, require more than one electron to map the position of an atom's electrons. Hydrogen has only one electron, so researchers often use hydrogen's nearest neighbor lithium, which has three electrons, to further their understanding of the nature of hydrogen compounds.

The team's results for lithium nitride showed the first experimental evidence that this compound undergoes a phase transition near 395,000 atmospheres of pressure. "The transformation represents a state that is uncommonly stable and compressible up to at least 2 million atmospheres of pressure," says Lazicki. "Lithium nitride is also one of the most difficult materials to metallize, with the metallization transition predicted to occur at 80 million atmospheres of pressure."

Maddox notes that although he works with an experimental group at Livermore, his advisors at Davis are theoretical physicists working on computational models. Maddox and Lazicki's data are useful feedback for their studies.

Maintaining Vision of Excellence

Over the years, the SEGRF Program has provided hundreds of young scientists and engineers a springboard to their professional careers. In exchange, the students have helped vitalize the Laboratory's research efforts and conducted studies of important fundamental science.

After graduation, many of the students remain at Livermore to contribute toward its national security missions. Dickinson notes, "The program has proven to be an important recruiting vehicle for building and maintaining scientific and engineering excellence at Livermore."

—Gabriele Rennie

Key Words: bioaerosol mass spectrometry (BAMS) system, Department of Applied Science (DAS), diamond anvil cell (DAC), homogenous charge compression ignition (HCCI), matrix-assisted laser desorption ionization (MALDI), neutron spectrometer, potassium dihydrogen phosphate, Qbox, Student Employee Graduate Research Fellowship (SEGRF) Program, ultrawideband (UWB) communications.

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Lawrence Livermore National Laboratory

The Best and the Brightest

Fewer than 1 percent of applicants become Lawrence fellows at Livermore.

Shea Gardner Kenneth Kim

Andrew Williamson

OULD you apply to be a Lawrence fellow, knowing your chances were less than 1 in 100 of being accepted? For the applicants, the stakes are high. But the payoff is great for both the fellows and the Laboratory.

This postdoctoral program is formally known as the Lawrence Livermore Fellowship Program. Informally, it is called the Lawrence Fellowship in tribute to Ernest O. Lawrence, the cofounder of the Laboratory, who cultivated creativity and intellectual vitality in the scientists who worked with him. Lawrence Livermore National Laboratory strives to do the same.

The Laboratory has always been a place where postdoctoral fellows thrive. They can work on state-of-the-art equipment with leaders in their field, performing research in areas of high demand. While all postdoctoral fellows pursue independent research, most are hired by a particular program, usually to perform research for a specific project. Lawrence fellows have no programmatic responsibilities and are given the opportunity to select the group in which they want to work. The allure of freedom and an atmosphere that cultivates creativity, coupled with a competitive salary and Livermore's extensive resources, make the Lawrence Fellowship Program a prestigious opportunity. In exchange, it brings to Livermore some of the most soughtafter Ph.D.s in the world.

The fellows produce remarkably creative research during their tenure. Many stay on as full-time career employees, continuing their work. Some leave Livermore to take positions at other institutions. But, as one fellow says, "The ones who leave are ambassadors for Livermore for the rest of their careers."

Solution to a Challenge

The Lawrence Fellowship Program was the brainchild of Jeff Wadsworth, former deputy director for Science and Technology. He initiated the program in 1997 in an effort to reverse the effects of the "dot-com" boom, which was leading many young scientists to choose the remuneration offered by private industry over employment with Department of Energy laboratories.

To help persuade the best and the brightest to come to Livermore, the Lawrence Fellowship offers an attractive salary and considerable research freedom. It was modeled after the J. Robert Oppenheimer Postdoctoral Fellowship Program at Los Alamos National Laboratory. In both programs, non-U.S. citizens may apply. Lawrence fellows are hired by the Director's Office, in cooperation with Livermore's University Relations Program.

The new program was first announced in the fall of 1997. Although some Lawrence fellows learn about

Julio Camarero

the program through contacts with Laboratory employees, most applicants find out about it through advertisements in journals such as *Science* and *Nature* or on the Web at either fellowship.llnl.gov/ or www.llnl.gov/postdoc/.

"We are interested in finding people who weren't necessarily thinking about coming to Livermore or who didn't know about Livermore initially," says Harry Radousky, chair of the Lawrence Fellowship Program committee.

The fellows are chosen for 3-year appointments by a selection committee consisting of a representative from each of the Laboratory's scientific directorates. The criteria for acceptance are rigorous. Out of 1,849 applicants in the first 4 years of the program, only 15 have been accepted. More recently, 282 applications were received for the program's fifth year, and 2 applicants have been invited to participate.

Each application is read by the selection committee, which looks primarily for leadership of stellar research projects. Applicants must have received their Ph.D. within the last 5 years. The applicant pool is eventually reduced to 6 individuals who undergo a 2-day interview. On the first day, the fellowship finalist gives a seminar on his or her area of interest; has lunch with the committee, which serves as a question-and-answer session; and then meets with current fellows in the afternoon. On the second day, applicants have the opportunity to talk to Laboratory scientists with whom they might be interested in working.

The goal of this process is to find people who will succeed at the Laboratory. The likelihood of success is measured in several ways: by matching an applicant's field of interest with



those of the Laboratory, examining the applicant's academic record and publications, and analyzing the research projects the applicant has initiated and the level of innovation those projects represent.

"We're not looking for management skills but at scientific leadership," says Radousky. "The object of the fellowships is to encourage intellectual vitality at the Lab and to recruit the best people in the world," he continues. "What we've discovered is that the application process is an excellent way to attract people to all kinds of positions. Many applicants who don't get into the Lawrence Fellowship Program are awarded postdoctoral fellowships to work in Laboratory programs or are hired as full-time employees."

Of the 15 individuals who have received Lawrence Fellowships thus far, 3 are now career employees, 2 left to become professors at the Massachusetts Institute of Technology (MIT), 1 went to the National Institute for Standards and Technology, another returned to his native Belgium, and the remaining 8 are still Lawrence fellows.

The Results of Freedom

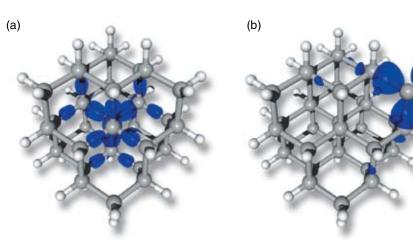
Freedom to work on projects and with mentors of their choice is what most current Lawrence fellows say attracted them to the program. This freedom, coupled with the Laboratory's interdisciplinary atmosphere, also

permits many fellows to move outside their initial area of specialization and investigate other scientific fields.

Wei Cai, for instance, a current Lawrence fellow from China, earned his Ph.D. from MIT. Midway through his graduate work, mentor Vasily Bulatov left MIT for the Laboratory. Bulatov encouraged Cai to apply for the program. Cai was a successful fellowship applicant and has worked not only with Bulatov but also with Malvin Kalos, the father of quantum Monte Carlo simulations. With Kalos, Cai has been investigating how to use Monte Carlo simulation codes more efficiently for modeling the microstructures of materials. Cai has amended some of Kalos's techniques and applied them to small-scale problems with great success. Now, together with Kalos, Bulatov, and other Livermore researchers, Cai is working on a project funded by the Laboratory Directed Research and Development

(LDRD) program to apply these techniques to larger, more complex systems. Cai has also been working on a new massively parallel computer code for modeling dislocation dynamics. "What happened here has a lot to do with the academic freedom the fellowship provides," Cai attests.

This freedom also allowed Cai to work on a particularly exciting project far removed from his usual line of research. At the suggestion of Giulia Galli, leader of the Quantum Molecular Dynamics Simulations Group, Cai tried to solve a problem that Galli's group was facing: adding a means of modeling a magnetic field to the electronic structure simulation codes regularly used to model condensed matter systems. Cai devised a code that successfully modeled in two dimensions the behavior of small systems, such as isolated hydrogen atoms and molecules, under an arbitrary magnetic field. The next step will be



Lawrence fellows Jeffrey Grossman and Andrew Williamson are using quantum Monte Carlo simulations to research the characteristics of nanostructures such as these silicon quantum dots. (a) A 71-atom silicon quantum dot. Hydrogen atoms (white) bonded to the surface make the material less reactive. (b) When a more reactive oxygen atom replaces two hydrogen atoms, the electron charge cloud (purple) is drawn toward the oxygen atom, dramatically changing the optical properties (wavelength) of the silicon quantum dot.



to apply this method with the more powerful electronic structure codes used for large-scale calculations, such as the modeling of magnetic field effects on the dynamics of fluid hydrogen.

Cai notes that the freedom allowed in the Lawrence Fellowship Program can be almost disconcerting at times. "You need discipline and must be able to make decisions at critical times about what you want to study."

Working at the Nanoscale

Two computational physicists became a team as Lawrence fellows. Jeffrey Grossman, a Ph.D. from the University of Illinois at Champaign-Urbana, and Andrew Williamson, a Ph.D. from the University of Cambridge in England, had known each other for years and both were interested in working with Giulia Galli. Almost immediately after arriving at Livermore as fellows, they applied for LDRD funding to use quantum Monte Carlo simulations to learn more about the characteristics of nanostructures, atomic-scale dots 1,000 times smaller

than the width of a human hair. (See *S&TR*, April 2002, pp. 4–10.)

"Scientific interest in nanotechnology centers around one very simple concept," says Grossman. "When you make something really small, its characteristics change. At the nanoscale—just a few hundred atoms—a material's properties start changing and become really interesting. Those differences and the ability to control the size of the structures mean that all kinds of new devices could be made—new ways to deliver drugs, storage systems for hydrogen fuel, detectors that can recognize microscopic amounts of anthrax in the air."

Livermore's supercomputers were a major draw for this duo because quantum Monte Carlo simulations are computationally intensive. With Livermore's computers, they can do work that they couldn't do at most places.

Another selling point was that Galli's group was beginning a new project on nanoscience when Grossman and Williamson joined the Laboratory. "Part of what makes the Lawrence Fellowship Program so attractive," says Williamson, "is the opportunity to create something new and shape the direction that research takes, rather than trying to come in and fit into a slot that was shaped by someone else."

Experimental biologist Julio Camarero, who is also working at the nanoscale, saw the Lawrence program advertised in *Science* and *Nature* while a postdoctoral fellow at Rockefeller University in New York City. Camarero received his Ph.D. from the University of Barcelona.

At Livermore, he started out in the Biology and Biotechnology Research Program (BBRP) but moved to the Chemistry and Materials Science Directorate, where he continues to perform biological experiments. He is a member of a team that aims to use dip-pen nanolithography to create and probe ordered arrays of proteins and colloids. One of the many uses for dip-pen nanolithography is to create tiny sensors that will detect biological warfare agents.

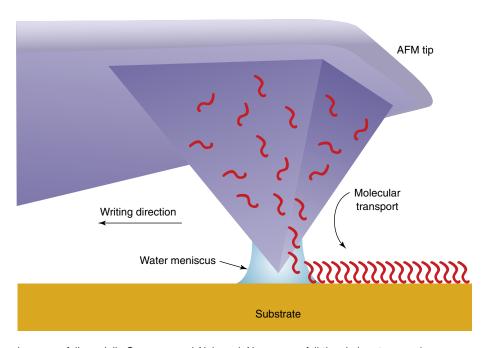
"The Lab is interested in applying science and technology to create tools for national security," notes Camarero. "I think that the technology we have developed is very powerful and has many applications, not the least of which is protecting us from biological terrorism."

In dip-pen nanolithography, the tip of an atomic force microscope is dipped into either an organic or inorganic substance (the "ink") and then is used to "write" on the surface of an inorganic substrate. (See *S&TR*, December 2001, pp. 12–19.) As the tip moves across the surface, it creates a precise, orderly pattern, or template, of material that is in chemical contrast to the substrate surface.

The goal of Camarero's research is to form specific chemical patterns less than 10-nanometers wide on silicon dioxide and gold surfaces. The chemicals in this template will react with proteins, thus making the template a sort of "molecular Velcro" to which the proteins bind in ordered arrays. Use of these templates allows for total control over the orientation of the proteins.

Small, Complex Systems

Kenneth Kim was at the University of Cambridge as a Wellcome Trust



Lawrence fellows Julio Camarero and Aleksandr Noy—now a full-time Laboratory employee—are pursuing research using dip-pen nanolithography. This technology uses the tip of an atomic force microscope (AFM) dipped in molecules to "write" on an inorganic substrate. The molecules react with the substrate to create a pattern of nanostructures attached to the substrate. These nanostructures have a variety of scientific uses.

fellow in the Applied Mathematics and Theoretical Physics Department when he learned about the Lawrence Fellowship Program from colleagues at the University of California at Berkeley and from Livermore's Web site. Kim works in BBRP's Computational and Systems Biology Division, led by Michael Colvin. "Traditionally, biology has been a qualitative discipline," Kim says. "But mathematics can play an important role in the biological sciences by providing a precise and powerful language to clarify underlying mechanisms and reveal hidden connections between seemingly disparate systems. Mathematical modeling may allow biology to become a predictive science alongside physics and chemistry."

Kim is applying the mathematical methods of statistical mechanics to the study of the astonishingly complex interactions and collective behavior of biological systems. He has studied the collective behavior of interacting bodies (inclusions) in an elastic medium (a cell membrane). The mathematical model that describes this behavior can be used to investigate the mechanism



that causes protein inclusions in cellular membranes to distribute themselves into large, stable aggregates as a function of their global shape. This research illustrates the rich interplay between geometry and statistical mechanics that underlies biological and other complex systems.

Kim is also developing a mathematical model for gene regulatory networks. In a gene network, the protein encoded by a gene can regulate the expression of other genes, which in turn control other genes. A protein can also regulate its own level of production through feedback processes.

"This network of interacting genes is another concrete example of collective behavior exhibiting an amazing degree of complexity at many spatial and temporal scales," says Kim.

Olgica Bakajin of Yugoslavia is yet another fellow working at the nanoscale. Bakajin had completed her Ph.D. at Princeton University and was on her way to the National Institutes of Health (NIH) when Livermore called to inform her that she was a successful Lawrence fellow applicant. Since arriving at Livermore, she has worked on several projects related to the development of novel microstructures and nanostructures. She is designing and fabricating a fast microfluidic mixer for the study of proteins. Just 10 micrometers wide-a human hair is 80 micrometers wide—the mixer can cause proteins to fold and unfold when solution conditions in the mixer are changed quickly and precisely. Bakajin will be using the mixer to examine the kinetics of fast protein folding reactions (an LDRDfunded project) and to investigate the kinetics of the folding of single-protein molecules (a collaboration with NIH scientists).

Working with former Lawrence fellow Aleksandr Noy, Bakajin is using carbon nanotubes in microfabricated devices to separate biological molecules. In the future, these microdevices could be used as detectors of chemical and biological warfare agents. "The interdisciplinary atmosphere at the Lab has provided me with lots of research opportunities," says Bakajin. "Right now, I have more ideas for interesting projects than I have time to pursue them."

Here to Stay

Three former fellows are now fulltime Laboratory employees, having exchanged some of the freedom of the Lawrence Fellowship for a staff position.

Theoretical biologist Shea Gardner, who studied population biology at the University of California at Davis, worked initially on several computational biology projects, one of which was a mathematical model to tailor chemotherapy treatments for individual cancer patients. Treatment strategies are based on the kinetics of the patient's particular tumor cells. Gardner has filed a provisional patent for this modeling approach and has been contacted about commercially developing the software.

Gardner also worked on biostatistics for the analysis of gene microarrays. A microarray is a glass microscope slide covered with "spots," each occupied by a different gene. (See *S&TR*, March 2002, pp. 4–9.) The entire slide is exposed to a stimulus such as a chemical or a change of temperature, and scientists note how each gene responds to the stimulus. "With microarrays, you can see the expression of over 12,000 genes at once, in a single run," Gardner notes.

"Previously, you could look at just one gene at a time."

Gardner is now participating in bioinformatics work for the National Nuclear Security Administration's Chemical and Biological National Security Program, computationally identifying DNA signatures that could be used to detect biological pathogens. She hopes to continue with this research. "Mathematical modeling, biostatistics, and bioinformatics are really different," she says. "Where else would I have had the opportunity to work on all three?"

Aleksandr Noy, a physical chemist from Harvard University, came to Livermore in 1998 to work on high-resolution microscopy. To that end, he developed a new microscope system that combines the topographic capabilities of the atomic force microscope with the spectroscopy capabilities of a confocal microscope. (See *S&TR*, December 2001, pp. 12–19.)

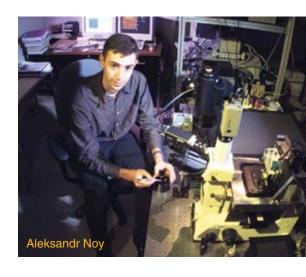
"My interests morphed from just looking at tiny things to fabricating them and using them for nanoscience applications," he says. "Shifting focus like that would not have been possible if I had not been a Lawrence fellow." Noy has worked on several nanoscience projects, including some that use carbon nanotubes in unique ways. Much of his research requires his new microscope to make the results visible.

He now leads a group that is fabricating electroluminescent nanostructures by dip-pen nanolithography. The researchers "write" with a conjugated polymer that emits light when a voltage is applied. Nanowires made of conjugated polymer poly [2-methoxy, 5-ethyl [2' hexy(oxy)] para-prenylene vinylene], or MEH-PPV, may some day serve as

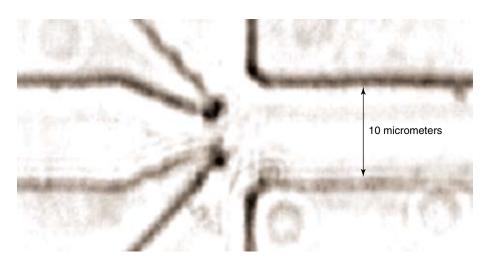
light-emitting nanodiodes. MEH-PPV nanowires are also highly sensitive to light and can serve as tiny optoelectric switches, which today are typically 1,000 times larger than tomorrow's MEH-PPV nanowires will be.

Plasma physicist Robert Heeter heard about the Lawrence Fellowship Program from Paul Springer, a group leader in Livermore's Physics and Advanced Technologies Directorate, who performs laboratory astrophysics experiments. Heeter has been working with Springer since coming to Livermore in 1999.

While at Princeton University earning his Ph.D., Heeter worked in England at the Joint European Torus, a magnetic fusion energy facility. But because of funding cuts, magnetic fusion research had fewer opportunities when Heeter was about to graduate. He was also interested in astrophysics, so he decided to apply for a Lawrence Fellowship at Livermore, which had active programs in both astrophysics and fusion energy.



Heeter became a Lawrence fellow and almost immediately got involved in photoionization experiments on Sandia National Laboratories' Z Accelerator in Albuquerque, New Mexico. Today, he continues his photoionization research. "I've also been doing other experiments in high-energy-density plasma physics," he adds. "I've stayed in the same group and in the same field that I was in as a fellow. High-energy-density physics experiments have numerous

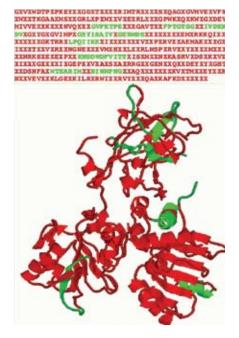


Olgica Bakajin is designing and fabricating this fast microfluidic mixer used for researching the kinetics of protein folding.

applications: in stockpile stewardship, in inertial fusion, and in astrophysics. And there's a lot of fundamental science to explore that hasn't been done before."

Laboratory Ambassadors

Not all Lawrence fellows stay on as full-time Laboratory employees. The most recent one to depart was metallurgist Christopher Schuh, who left in the summer of 2002 to become



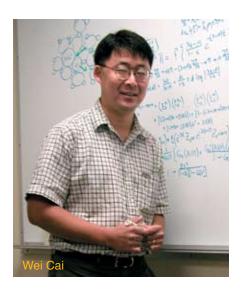
One of the research interests Shea Gardner pursued as a Lawrence fellow, which she continues today as a Laboratory employee, is modeling the DNA signatures of viral pathogens. These simulations contribute to technologies for detecting agents of biowarfare.

a professor at MIT. After completing his Ph.D. at Northwestern University, he came to Livermore to work on grain boundary engineering, in which conventional metallurgical processing is tailored to produce better metals. Grain boundaries—where crystals with different orientations come together—are the weak link in any material. Schuh examined ways to manipulate the orientation of crystals at grain boundaries to create metals with desirable properties such as less cracking, corrosion, and cavitation.

Schuh's research also took him beyond grain boundaries to the individual atoms in the crystals. "If you disturb the atoms in metals so much that the crystal structure no longer looks anything like that of traditional metals, the metals will have very different properties," said Schuh. "We're trying to understand how these changes affect the physics of the metal."

Schuh notes that postdoctoral fellows typically join a program with the understanding that they have been hired to work with someone on a certain project. "For Lawrence fellows," he says, "there's no such obligation. That gives you complete freedom and a lot of latitude."

Nicolas Hadjiconstantinou received his Ph.D. from MIT and immediately joined Livermore as a Lawrence fellow, deferring a teaching appointment at MIT for a year. While at Livermore, he helped to develop a code that extended the use of direct Monte Carlo



calculation from the simulation of dilute gases to the simulation of dense fluids. With this code, Livermore researchers can simulate for the first time the phase change characteristics of a van der Waals fluid.

Joel Ullom, who completed his Ph.D. at Harvard, focused on the development of cryogenic detectors, which are small electrical circuits that produce a current or voltage pulse when hit by a photon or particle. The detector must be cooled to temperatures between 0.1 and 1-kelvin, so that the energy of a single photon will produce measurable heating. Ullom used cryogenic detectors to weigh the protein fragments dislodged from bacterial spores by a pulse of laser light. He also developed refrigeration technology to produce the ultralow temperatures needed for cryogenic detectors. Ullom became a Laboratory

career employee before leaving for a position at the National Institute of Standards and Technology.

Luc Machiels, a native of Belgium, received his Ph.D. from the Swiss Federal Institute of Technology. After a postdoctoral position at MIT, he came to the Center for Applied Scientific Computing, where he solved problems in continuum mechanics. With colleagues at MIT, he developed a new finite-element error control strategy for the version of the Navier–Stokes equation that describes the motion of an incompressible fluid. The technique, which is both accurate and efficient, calculates lower and upper limits for the output of a system, such as the temperature bounds at the surface of an electronic device. Before leaving Livermore, he also developed new techniques for the solution and modeling of partial differential equations.

A Resounding Success

Radousky has only good things to say about the Lawrence Fellowship Program. "We've learned that we can attract really top people to the Laboratory," he says. "This program has attracted the best young scientists to the Lab and promoted university collaborations. It is also an excellent way to do general recruiting."

When the program first started, more fellows were engaged in traditional physics research, while today more are studying biology and nanoscience. This shift is consistent with changes throughout the scientific

community. Biological research leaped to the foreground with the success of the Human Genome Project. Many experts predict that the 21st century will be remembered for a revolution in biotechnology and medicine comparable to the advances made during the last century in physics.

Nanoscience is a similarly "hot" research topic. As all kinds of devices in our world become smaller and smaller, nanostructures of all types will find many uses.

All in all, the Lawrence Fellowship Program has been a resounding success in bringing new talent to the Laboratory and encouraging creativity and exciting science.

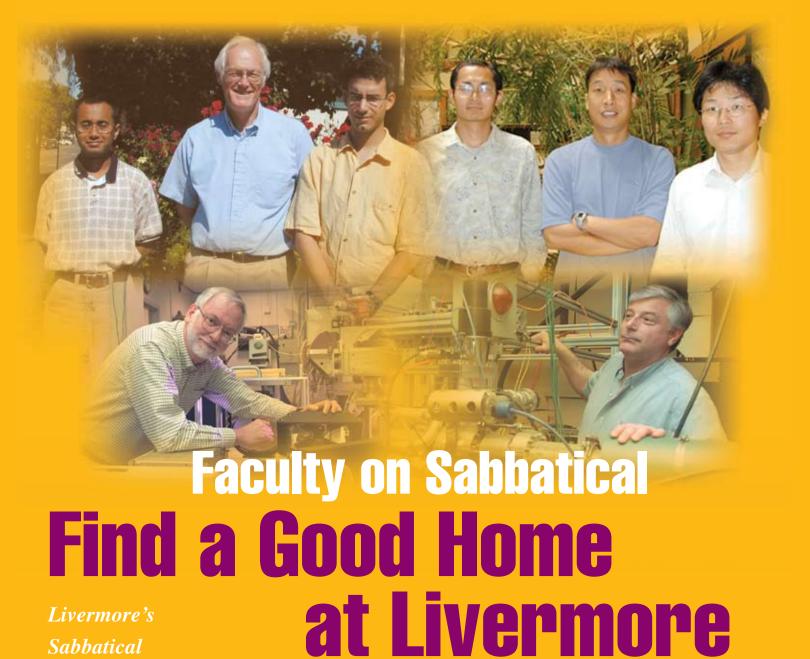
-Laurie Powers and Katie Walter

Key Words: Lawrence fellows, Lawrence Fellowship Program, postdoctoral positions.

For further information contact Harry Radousky (925) 422-4478 (radousky1@llnl.gov).

For information on the Lawrence Fellowship Program and other fellowship opportunities at the Laboratory, see these Web sites:

fellowship.llnl.gov/ www.llnl.gov/postdoc/



Livermore's
Sabbatical
Scholars Program
is attracting
top academic
scientists and
their students to
the Laboratory.

OR university faculty members, a sabbatical leave is one of the most valued perks of academic life. Typically, a sabbatical means an opportunity every seventh year to conduct research for several months, or sometimes a full academic year, without a teaching workload. An increasing number of faculty members are choosing to spend their sabbaticals at Lawrence Livermore.

Livermore's Sabbatical Scholars
Program was designed to bring topflight
scientific and engineering expertise to the
Laboratory. This program gives visiting
professors the opportunity to conduct
research at one of the world's premier
applied science and engineering research
centers, and Livermore scientists have the
opportunity to collaborate with some of
the best scientific minds in the world. The

established ties serve to strengthen the recruitment of outstanding young scientists and engineers.

"Our sabbatical program is a costeffective way to take advantage of the outstanding scientists in the nation and the world," says Harry Radousky, deputy director of Livermore's University Relations Program (URP). URP was formed in 1995 to facilitate the growing number of collaborations between Laboratory researchers and academic institutions. "Strong interactions between the university community and Lawrence Livermore are vital to the continuing success of the Laboratory's missions," says Radousky. (See *S&TR*, October 2004, pp. 14–23.)

URP advertises the program annually in science journals, such as Science and Nature, and through promotions on selected university campuses, particularly those in the University of California (UC) system. In many cases, Laboratory researchers encourage their university collaborators to apply.

Painless Application Process

"We try to make the application process as painless as possible," says URP's Paul Dickinson, who manages the Sabbatical Scholars Program. Applicants fill out an interest form located on URP's Web site and submit a curriculum vita and brief description of the research they propose to conduct at Livermore. According to Dickinson, some applicants have already collaborated with Livermore researchers, know one or more Livermore scientists. or have visited the Laboratory. Others are attracted by Livermore's reputation in applied science and engineering.

Applications are due May 1 each year, but they are reviewed quarterly until available resources are committed. Applications are first screened by the potential host Laboratory directorate to determine if there is a good match for the applicant and a Livermore program that would benefit from the sabbatical.

Applications are then formally reviewed by the same Laboratory-wide committee that selects the Lawrence Fellows (outstanding postdoctoral scholars; see S&TR, November 2002, pp. 12–21). Sabbatical candidates are evaluated on their records of achievement and the strength of their research proposals. The committee ranks all applicants and chooses four to six faculty members per fiscal year for sabbaticals that can range from 3 to 15 months.

A unique feature of the program is the inclusion of graduate students and postdoctoral researchers in a faculty member's sabbatical stay at the Laboratory. "Encouraging faculty to bring outstanding students and postdocs with them has proved to be very popular," says Dickinson. The number of students and the duration of their visit to Livermore are negotiated with each faculty participant. Dickinson explains that when faculty members return from a typical sabbatical, they have to "restart" their students' research programs. Under the Livermore program, students return to campus with little break in continuity of their studies.

Since the program's inception in 2000, 22 faculty members have been Livermore Sabbatical Scholars, and 33 of their students and postdoctoral researchers

have joined them at Livermore. Faculty members have come from universities throughout the U.S. as well as France, Italy, the Netherlands, and Japan. Six of the 22 professors have come from the UC campuses at Berkeley (UCB), Davis (UCD), and Riverside (UCR). (See the box on p. 34.)

Livermore program directorates have been extremely pleased with the facultystudent teams that the Sabbatical Scholars Program has attracted. "In many cases, faculty-student teams working at the Laboratory for 3 to 12 months have made significant contributions to our technical programs or helped establish new capabilities," says Dickinson. "In most instances, collaborations were established that continue to grow in scope."

The program has also proven to be cost-effective. In most cases, faculty on sabbatical have some fraction (often 80 to 100 percent) of their salary paid by their home institution. As a result, Livermore's costs are usually limited to temporary housing and travel expenses for the professor and any students.

First Sabbatical Scholar

Richard Martin, professor of physics at the University of Illinois at Urbana-



In 2001, University of Illinois physicist Richard Martin (center) was the first participant in the Laboratory's Sabbatical Program. **During Martin's** sabbatical, three of his graduate students visited Livermore for extended periods, and two of his postdoctoral researchers (shown here with Martin) made short visits.

Champaign, was the first program participant, with a 14-month sabbatical that began in July 2001. At its conclusion, he characterized his sabbatical as "a stimulating, profitable, and enjoyable experience."

Martin, an expert on the electronic properties of solids, proved how

productive a sabbatical at Livermore could be. Martin's hosts were physicists Andy McMahan and Giulia Galli in the Physics and Advanced Technologies (PAT) Directorate's H Division, which researches the behavior and structure of materials under extreme conditions. Martin was located in the Laboratory's

Materials Research Institute (MRI), where he could interact with a wide range of Livermore scientists.

Martin worked with McMahan and physicists David Young and Jim Albritton on improving quantum models used to generate equations of state. In another project, Martin and McMahan researched

Name	University	Dates onsite	Students/ postdocs	Host directorate	Host
Richard Martin	University of Illinois, Urbana-Champaign	07/01–08/02	5	Physics and Advanced Technologies	Giulia Galli, Andy McMahan
James Hunt	University of California, Berkeley	09/01–08/02	2	Energy and Environment/ Chemistry and Materials Science	Ken Jackson, Jesse Yow
James Orr	University of Pierre and Marie Curie (France)	09/01–08/02	2	Energy and Environment	Ken Caldeira
Joonhong Ahn	University of California, Berkeley	01/02-10/02	2	Energy and Environment	Bill Halsey
Herbert Edelsbrunner	Duke University	01/02-06/02	2	Computation	David Keyes
James Carlson	University of California, Davis	04/02-06/02	1	Physics and Advanced Technologies	Steve Visuri
Carlo Bottasso	Politecnico di Milano (Italy)	06/02-11/02	2	Engineering/Computation	Dennis Parsons
Stanley Prussin	University of California, Berkeley	08/02-05/03	2	Nonproliferation, Arms Control, and International Security	Tom Gosnell
Stephen Park	University of California, Riverside	09/02-05/03	0	Energy and Environment	Jeff Roberts
Joyce Penner	University of Michigan	09/02-09/03	3	Energy and Environment	Doug Rotman
Peter Pacheco	University of San Francisco	09/02-05/03	1	Computation	Patrick Miller
James Badro	University of Pierre and Marie Curie (France)	12/02-03/03	0	Energy and Environment	Daniel Farber
R. Paul Drake	University of Michigan	01/03-09/03	2	National Ignition Facility Programs	Bruce Remingto
Michael Walter	Okayama University (Japan)	01/03-03/04	0	Chemistry and Materials Science	Joseph Zaug
John Trangenstein	Duke University	01/03-05/03	2	Computation	Richard Hornung
Alexander Tielens	Kapteyn Astronomical Institute (Netherlands)	06/03-08/03	3	Physics and Advanced Technologies	Wil van Breugel
J. Ilja Siepmann	University of Minnesota	08/03-07/04	1	Chemistry and Materials Science	Chris Mundy
George Hepner	University of Utah	10/03-02/04	1	Energy and Environment	Bill Pickles
James Brennan	University of Toronto	03/04-05/04	0	Energy and Environment	Rick Ryerson
Edison Liang	Rice University	03/04-08/04	2	National Ignition Facility Programs	Bruce Remingto
Edward Morse	University of California, Berkeley	09/04–05/05	0	National Ignition Facility Programs/ Physics and Advanced Technologies/ Nonproliferation, Arms Control, and International Security	Mike Moran
Scott Davis	Naval Postgraduate School	10/04-03/05	0	Nonproliferation, Arms Control, and International Security	Bill Conaway

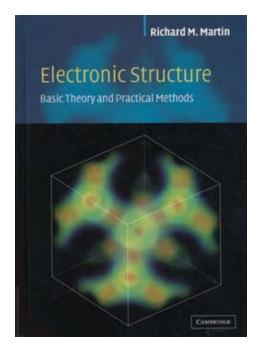
strong electron correlation, a phenomenon encountered in some materials of Laboratory interest. In these materials, one cannot make the assumption that each electron in a solid interacts independently of all the other electrons. Martin also worked with physicists Andrew Williamson, Jeff Grossman, Galli, and others on Monte Carlo simulations and time-dependent density functional theory. Adding time dependence improves modeling capabilities based on this theory, such as the ability to predict energy gaps in solids.

Three of Martin's graduate students visited Livermore for extended periods, and two of his postdoctoral researchers made short visits. Martin started an ongoing collaboration that included one of his students with physicist Mal Kalos of the Defense and Nuclear Technologies Directorate.

During Martin's stay, he also completed the book *Electronic Structure*: Basic Theory and Practical Methods, which was recently published by

Cambridge University Press. "One outcome of Richard's many interactions with Laboratory staff was he became a member of the H Division Advisory Committee. He continues to visit the Laboratory about twice a year to sit on this oversight panel that assesses the division's progress," says McMahon.

Sabbatical scholars who have followed Martin include climate experts, nuclear physicists, engineers, computer scientists, and chemists. James Orr, an oceanographer whose research focuses on the cycling of carbon within the ocean and the exchange of carbon between the atmosphere and ocean, completed a yearlong sabbatical in 2002. Orr is a scientist with the Laboratoire des Sciences du Climat et de l'Environment of the French Commissariat à l'Energie Atomique and the l'Institut Pierre-Simon Laplace. He is the international coordinator of the Ocean Carbon-Cycle Model Intercomparison Project, which compares and improves three-dimensional numerical models of the ocean.



During physics professor Richard Martin's sabbatical, he completed the book *Electronic* Structure: Basic Theory and Practical Methods, which was recently published by Cambridge University Press.



Joonhong Ahn (left), associate professor in the Department of Nuclear Engineering at the University of California at Berkeley, spent a nine-month sabbatical at Livermore in 2002 with two of his graduate students. The three researchers studied the relationship between the nuclear fuel cycle and geologic disposal.

During his sabbatical, Orr worked with Livermore's Climate and Carbon Cycle Group in the Atmospheric Sciences Division of the Energy and Environment Directorate to achieve the highest resolution simulations of carbon transport with an atmospheric model that had yet been produced. This work led to new projects funded by the National Aeronautics and Space Administration and the Department of Energy (DOE). A strong collaboration continues between Livermore and Orr's group in France.

Joonhong Ahn, associate professor in nuclear engineering at UCB, spent a nine-month sabbatical at Livermore in 2002. Ahn and two of his graduate students studied the relationship between the nuclear fuel cycle and geologic disposal. Their work led to the development of a nuclear fuel cycle mass-flow model for transmuting wastes with an accelerator. Ahn's sabbatical resulted in an expanded

collaboration between Livermore and UCB's Department of Nuclear Engineering.

From Scholar to Chief Scientist

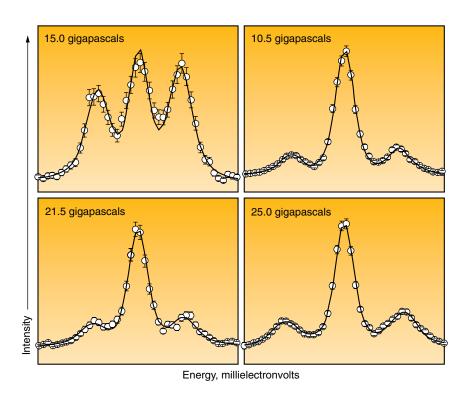
Another member of UCB's Department of Nuclear Engineering, Professor Stanley Prussin, had served for several years as a consultant to Livermore's Nonproliferation, Arms Control, and International Security (NAI) Directorate before his sabbatical from August 2002 to May 2003. During his Livermore sabbatical, Prussin became interested in a Laboratory Directed Research and Development (LDRD) project to develop a method for detecting the clandestine transport of nuclear weapons materials inside shipping containers. The challenge for NAI was to detect a very small amount of highly enriched uranium or plutonium buried inside a typical freight container. Such a detection system is required at the nation's seaports because currently only

2 percent of nearly 7 million shipping containers that enter the U.S. are inspected.

NAI physicist Tom Gosnell, who was Prussin's host, recalls Eric Norman of Lawrence Berkeley National Laboratory visiting Prussin at Livermore. Gosnell observes, "When you give two really smart guys an office and time to think, they can come up with great things." Prussin and Norman were instrumental in developing a detection system that may be 10,000 times more sensitive than other approaches under certain conditions. The system bathes suspicious containers with neutrons to actively search incoming shipments for smuggled nuclear materials. Prussin is currently project chief scientist. (See *S&TR*, May 2004, pp. 12–15.)

Two graduate students accompanied Prussin. One of them, Dave Peterson, was awarded a Student Employee Graduate Research Fellowship (SEGRF).

Livermore physicist Daniel Farber and geophysicist James Badro, a sabbatical scholar from the Institut de Physique du Globe de Paris. France, have advanced scientific understanding of inelastic x-ray scattering of crystals, which measures a crystal's vibrations. These plots show some of the highest pressure and highest resolution single-crystal phonon dispersion (crystal lattice vibration) data ever collected. A beam of 20,000 electronvolts was directed in a longitudinal direction (left column) and then a transverse direction (right column) on a crystal of cobalt. The researchers recorded tiny (about 10-millielectronvolt) shifts in the crystal's vibrational energy, seen in the left- and right-hand peaks flanking the large central peak in each graph.



Livermore's URP, in partnership with UC, provides these 4-year fellowships to students pursuing a Ph.D. at UC who are conducting their thesis research at the Laboratory. In 2004, there were about 50 SEGRF students at Livermore.

James Carlson, associate professor in the Department of Medical Pathology in the School of Medicine, and director of the Clinical Microbiology Laboratory at UCD's Medical Center, completed a threemonth sabbatical at Livermore in 2002. He worked with Livermore's Medical Technology Program to define a project in the rapid diagnosis of respiratory viruses. While on sabbatical, he and one of his graduate students were able to carry out experiments using biomedical equipment developed at Livermore. Carlson is currently collaborating on a project funded by LDRD to develop a point-of-care pathogen-detection instrument.

Long-Term Collaboration

Geophysicist James Badro, from the Institut de Physique du Globe de Paris, France, was on sabbatical at Livermore from December 2002 to March 2003. His host was long-time collaborator Dan Farber, a high-pressure physicist in the Earth Sciences Division in the Energy and Environment Directorate. The two first met in Europe in 1994 at a conference. Two years later, Farber came across one of Badro's research papers. "It was one of the few times I've been stunned by a scientific paper," he says.

Later, Farber and Badro worked together for two years at the European Synchrotron Radiation Facility (ESRF) studying inelastic x-ray scattering of crystals. "We developed a technique that measures the modes of vibrations in crystals," says Farber. The work paved the way for a team that included Farber and was led by Livermore chemist Joe Wong to study phonon dispersions (crystal lattice vibration) of plutonium

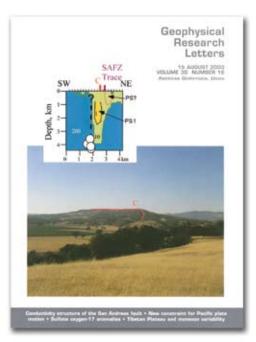
at ESRF. The team, funded by LDRD, produced new phonon data that greatly enhanced scientists' basic knowledge of the phases of plutonium. (See S&TR, January/ February 2004, pp. 12–14.)

Badro's sabbatical continued the work on inelastic x-ray scattering and allowed the two physicists to generate ideas for new research that take advantage of Livermore's capabilities. Badro has returned to the Laboratory several times since his sabbatical ended in 2003. He and Farber currently have a long-term project supported by the Livermore branch of UC's Institute for Geophysics and Planetary Physics. The project focuses on new ways to obtain data on high-pressure, high-temperature materials.

"Livermore is attractive to many faculty members," says Farber. "We have great technical capabilities, and the campus encompasses a broad range of interests. Faculty members can interact with people doing different things and that can generate new collaborations. The sabbatical program encourages visitors to share their ideas and techniques and allows us to stay engaged with the broader scientific community."

Stephen Park, professor of geophysics with the Department of Earth Sciences and a researcher in the Institute of Geophysics and Planetary Physics branch at UCR, completed a nine-month sabbatical at the Laboratory in the summer of 2003. He partnered with Livermore physicist Jeff Roberts on a project funded by LDRD involving electrical resistivity monitoring of the San Andreas Fault at Parkfield, California. The scientists measured electrical conductivity of sediments adjacent to the fault. The measurements suggested the active portion of the fault at Parkfield may be offset by as much as 1,000 meters from the mapped surface break. (See *S&TR*, March 2005, pp. 22–23.)

Michael Walter, professor from Okayama University, Japan, spent a



Geophysicist Stephen Park, a sabbatical scholar from the University of California at Riverside, partnered with Livermore physicist Jeff Roberts on a project involving electrical resistivity monitoring of the San Andreas Fault at Parkfield, California. Their work was reported in the August 15, 2003, issue of Geophysical Research Letters. (Copyright 2003 American Geophysical Union; reproduced by permission.)

13-month sabbatical (January 2003 through March 2004) that was jointly supported by Okayama University and Lawrence Berkeley and Lawrence Livermore national laboratories. Walter designed and constructed an advanced laser-heated diamond anvil cell (LHDAC) system for the new high-pressure beam line 12.2.2 at the Advanced Light Source (ALS) facility at Lawrence Berkeley, one of the world's brightest sources of ultraviolet and soft and hard x-ray beams.

A diamond anvil cell (DAC) is a small mechanical press that forces together the small, flat tips of two diamond anvils, thereby creating extremely high pressures on a tiny sample of a material. Using a laser is an effective way to heat DAC samples. The ALS beam line enables scientists to study the structure of the sample being squeezed and heated in the DAC.

Walter has shared his LHDAC expertise with researchers in Livermore's Chemistry and Materials Science Directorate. In March 2004, he demonstrated how the LHDAC system heats water to well over 2,000 kelvins. "Walter was instrumental in building a laser heating system at the ALS that will enable us to learn about materials using x-ray diffraction as a probe when sample conditions extend to 3,000 or 4,000 kelvins and over 100 gigapascals," says Livermore chemist Joe Zaug, who was Walter's host.

Current Scholars

The most recent sabbatical scholars-Edward Morse from UCB and Scott Davis from the Naval Postgraduate School (NPS) in Monterey, California—arrived at Livermore in the fall of 2004. Morse is the third faculty member from UCB's Department of Nuclear Engineering to participate in the sabbatical program. As a reflection of Morse's unusually broad research interests, his stay is supported by three directorates: National Ignition Facility (NIF) Programs, NAI, and PAT.

Morse has been involved with Livermore for several years. His graduate student, Carlos Barrera, is completing his Ph.D. researching NIF physics. Barrera, in February 2005, was awarded a fellowship at Livermore under the SEGRF Program. Morse is working with Mike Moran and other Laboratory laser scientists to develop a neutron imaging diagnostic for NIF. Morse has overseen tests of the new detector using neutrons generated at both Livermore and UCB facilities. He has also developed detectors that use diamonds to achieve unprecedented sensitivity. "We're

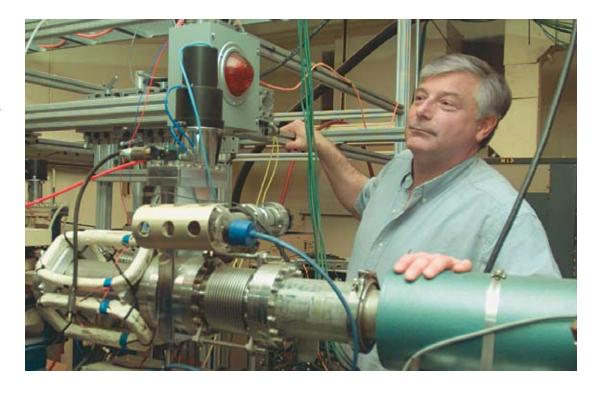
trying to design the diagnostics of the future," he says.

"Morse has been an important resource for us," says Moran, Morse's host. "He has maintained a relationship with Livermore that has evolved as our priorities, needs, and programs have evolved."

For PAT, Morse works closely with Livermore experts in neutron generation and detection. He runs a neutron generator at UCB that previously was located at Livermore. He is currently working with PAT managers on ways to make Livermore's Pelletron, a positron accelerator used to study radiation damage, available to UCB researchers. As an example of the close relationship between Livermore and UCB, Brian Wirth, a former Laboratory physicist, is the newest member of UCB's Nuclear Engineering staff and will oversee UCB access to the Pelletron.

Morse has developed a graduate-student course on nuclear nonproliferation for

Sabbatical scholar Edward Morse from the University of California at Berkeley (UCB) examines Livermore's Pelletron, a positron accelerator. Materials experiments will be performed on this accelerator by a UCB-Livermore team.



the Western Nuclear Science Alliance, a DOE-sponsored consortium of college nuclear engineering programs. The two-week course, Analytical Methods of Nonproliferation, was presented last fall at the Idaho National Engineering and Environmental Laboratory and will be taught this summer to between 20 and 40 students from across the nation by what Morse describes as a "dream team" of Livermore scientists.

"The course introduces graduate students to the key issues of nonproliferation issues and national policy," Morse explains. "I thought Livermore would be a good place to host the course," he says, adding that the course will serve as a way to attract talented graduate students to Livermore. Teaching will be coordinated by Simon Labov, director of the Laboratory's Radiation Detection Center.

Physics Professor Scott Davis works in atomic, molecular, and optical physics

to develop new generations of sensors at NPS for the Department of Defense. Davis says, "A few years ago, Bill Kruer from Livermore worked for a couple of years at NPS and planted a seed in my brain about spending some time at Livermore." Davis was already familiar with the Laboratory years ago, he had brought his graduate students to Livermore for a tour of the Nova laser.

After applying to the program, Davis was invited to Livermore to present a colloquium on ultraviolet (UV) imaging spectrometers developed at NPS. Davis arrived for a six-month stay in October 2004. He worked on two advanced remotesensing techniques that are part of NAI's efforts to detect clandestine weapons of mass destruction.

The first research effort was a collaboration with chemist Nerine Cherepy to develop UV imaging and spectroscopy methods to detect radionuclides in the

environment. This effort, funded by LDRD, takes advantage of the fact that alpha and beta particles cause UV fluorescence; that is, they glow in air. A UV imaging detection system could, for example, be used to assess and aid in the cleanup of an area contaminated by a "dirty bomb" or a radionuclide spill. Current experiments are being performed to evaluate airglow brightness for different response scenarios and to optimize detection efficiency.

A second effort Davis participated in investigated new types of infrared (IR) imaging spectrometers to identify chemical species at low concentrations in the atmosphere and quantify their concentrations based on their IR signatures. "IR signatures are generally specific to each type of molecule," says Davis. One aspect of the project explored new design options for a near-IR imaging spectrometer with higher resolving power than is available with current



Sabbatical scholar Scott Davis from the Naval Postgraduate School works in Livermore's infrared imaging spectroscopy laboratory.

models. A second aspect investigated the potential application of new detector technologies to long-wavelength IR imaging spectroscopy, an area in which Livermore is an acknowledged leader. IR imaging spectrometers mounted on ships, airplanes, or unmanned airborne vehicles might, for example, remotely detect and measure effluents from facilities and provide insight into whether the facilities were involved in the manufacture of nuclear or chemical weapons.

Davis's host in NAI, Bill Conaway, notes that Livermore's long-standing relationship with NPS was strengthened last April when U.S. Navy Rear Admiral Patrick Dunne and Laboratory Director Michael Anastasio signed a Memorandum of Understanding establishing a framework for stronger collaboration in the area of national security. Conaway says a short-term benefit from Davis's stay was cross-fertilization among scientists, while a long-term benefit was building bridges between Livermore and the NPS. "Scott has excellent students as well as experience with sponsors different from ours," says Conaway. "We want to continue the momentum that he began."

New Emphasis

With the Sabbatical Scholars Program in its fifth year, the benefits continue to grow. There are an increasing number of opportunities to recruit scientific and engineering talent from the graduate students and postdoctoral researchers accompanying faculty. Many of these researchers stay in contact with their Livermore hosts, some return to the Laboratory as part of continuing collaborations, and two have become Livermore employees.

"The Sabbatical Scholars Program has been enormously successful," says Radousky. "The benefits keep coming."

—Arnie Heller

Key Words: Advanced Light Source (ALS), European Synchrotron Radiation Facility (ESRF), laser-heated diamond anvil cell (LHDAC), Naval Postgraduate School (NPS), Sabbatical Scholars Program, University Relations Program (URP).

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